CRYSTALS OF THE ALPHA 1 BETA 1 INTEGRIN I-DOMAIN AND THEIR USE

RELATED APPLICATIONS

This is a continuation of PCT/US99/23261, filed on October 6, 1999 as a continuation of prior U.S. provisional Serial number 60/103,301, filed October 6, 1998. The entire disclosure of each of the aforesaid patent applications are incorporated herein by reference.

BACKGROUND OF THE INVENTION

A major class of cell receptors that interacts with the constituents of the extracellular matrix (" ECM") (e.g, collagen, laminin) are the integrins which are transmembrane heterodimeric glycoproteins composed of noncovalently associated α and β subunits. The integrin family contains at least 16 α subunits, seven of which contain an approximately 200 amino acid inserted domain in their N-terminal region variously called the "I-domain" or the "A-domain".

Processes such as cell differentiation, cell proliferation and cell migration in embryonic development, as well as remodeling and cell/tissue repair events, are dependent on communication of cells with the ECM. Alpha 1 beta 1 integrin ("α1β1 integrin") is a cell-surface receptor for collagen I, collagen IV and laminin. It is also known as VLA-1. Indeed, α1β1 supports not only collagen-dependent adhesion and migration, but also is likely to be a critical collagen receptor on mesenchymally-derived cells that may be involved in ECM remodeling after injury (Gotwals et al.(1996), J. Clin. Invest. 97 : p 2469-2477). The ability of cells to contract and organize collagen matrices is a critical component of any wound healing response. Improper regulation of α1β1 integrin may result in certain pathological conditions such as fibrosis.

Moreover, there is a limited, but provocative, literature suggesting that α1β1 may play a role in T cell/monocyte driven diseases. Anti-α1β1 antibodies block T-cell dependent cytokine expression. Miyake et al., J. Exp. Med., 177: 863-868 (1993). Expression of α1β1 is upregulated in persistently activated, 2-4 week old cultured T cells (Hemler et al., Eur. J. Immunol., 15: 502-508 (1985)) and is also expressed on a high percentage of T cells isolated from the synovium of patients with rheumatoid arthritis. Hemler et al., J. Clin. Invest., 78: 696-702 (1986). Chronic tissue damage results from both

resident activated T cells, and also monocytes/fibroblasts recruited by T cell-derived cytokines. Blocking the α1β1–induced T cell interaction might relieve tissue damage by removing activated T cells and/or by diminishing inflammatory cytokine levels.

It would therefore be useful to design, identify or obtain potential drug candidates which would interfere with the α1β1 integrin-ECM or T-cell interaction(s). The recent emergence of drug design to identify candidates that play a role in a physiologically relevant biological pathway has provided a useful approach for obtaining, or designing, lead compounds for drugs.

Generally, this approach requires selecting a protein target molecule which plays a role in a physiologically relevant biological pathway. Typically, once an inhibitor or agonist, natural or synthesized, is found for the target molecule, it is modified or optimized to produce a candidate with the desired properties.

In order to more efficiently design or modify a ligand, it is useful to have a three-dimensional structure for the bioactive conformation of a known ligand as it binds to the target protein molecule. Furthermore, it is valuable to understand the detailed interactions of the ligand with its target protein by examining the three-dimensional structure of the protein target in complex with its known ligand. This allows the artisan to preserve the critical interactions with the protein, while modifying candidate ligands to interact more precisely with the protein, resulting in better potency and specificity.

However, the three dimensional crystal structure of the protein target is frequently unavailable due to the significant effort required to obtain crystals of sufficient size and quality to provide accurate information regarding the structure. For example, it is time consuming and often difficult to express, purify and characterize a protein. Additionally, once the protein of sufficient purity is obtained, it must be crystallized to a size and quality which is useful for x-ray diffraction and subsequent structure solution. Thus, although crystal structures can provide a wealth of valuable information in the field of drug design and discovery, crystals of certain biologically relevant molecules such as α1β1 integrin, are not readily available to those skilled in the art.

Furthermore, although the amino acid sequence of a target protein, such as α1β1 integrin, is known, this sequence information does not allow an accurate prediction of the crystal structure of the protein. Nor does the sequence information afford an understanding

of the structural, conformational and chemical interactions between a ligand such as α1β1 integrin and its target.

Thus, there is a need for a detailed knowledge of the crystalline three-dimensional structure of the extracellular domain of α1β1 integrin, to effectively design, screen or optimize compounds capable of interfering with the α1β1 integrin-ECM and/or T-cell interactions.

A soluble version of α1β1 integrin can be made from its extracellular region or fragments thereof. As used herein, the term "α1β1 integrin" includes soluble α1β1 integrin polypeptides lacking transmembrane and intracellular regions, homologs and analogs of α1β1 integrin or derivatives thereof. Crystals of the α1 chain of α1β1 integrin or fragments thereof of a size and quality such as described herein, would allow performance of x-ray diffraction studies and enable those skilled in the art to conduct studies relating to the binding properties of α1β1 integrin, as well as the binding properties of molecules or molecular complexes which may associate with α1β1 integrin or fragments thereof.

SUMMARY OF THE INVENTION

Accordingly, the present invention is directed to crystals of the α1 chain of α1β1 integrin or crystals of fragments of the α1 chain, of sufficient size and quality to obtain useful information about the properties of α1β1 integrin and molecules or complexes which may associate with it. The claimed invention provides the three-dimensional crystal structure of the Cys143 to Ala340 fragment of the α1 chain of α1β1 integrin, which can be used to identify binding sites to solve the structure of unknown crystals, to provide mutants having desirable binding properties, and ultimately, to design, characterize, or identify molecules or chemical entities capable of interfering with the interaction between collagen or other ligands and α1β1.

Additional features and advantages of the invention will be set forth in the description which follows, and in part will be apparent from the description, or may be learned by practice of the invention. The objectives and other advantages of the invention will be realized and attained by the compositions and methods particularly pointed out in the written description and claims hereof, as well as in the appended drawings.

To achieve these and other advantages, and in accordance with the purpose of the invention, as embodied and broadly described herein, the invention relates to a crystal of α1β1 integrin. More particularly, the invention relates to a crystal formed by a functional

fragment of the extracellular domain of the α1 chain of α1β1(Cys143-Ala340), wherein the crystal has cell constants a= 34.77Å, b= 85.92Å, c= 132.56Å, α = β = γ =90Å, and a space group of $P2_12_12_1$, and equivalents of that crystal. The claimed crystals of α1β1 are substantially described by the structural coordinates identified in Table II. The claimed crystals in certain embodiments are characterized by a binding site moiety comprising Asp154, Ser156, Asn157,Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Mutants, homologs, co-complexes and fragments of the claimed crystals are also contemplated herein.

The claimed invention in certain embodiments relates to heavy atom derivatives of the crystallized form of α1β1 integrin (143-340), and, more specifically, the heavy atom derivatives of the crystallized form of α1β1 described above. In various embodiments, the claimed invention relates to methods of preparing crystalline forms of α1β1, or fragments thereof, by providing an aqueous solution comprising at least a fragment of α1β1, providing a reservoir solution comprising a precipitating agent, mixing a volume of the α1β1 solution with a volume of the reservoir solution and crystallizing the resultant mixed volume. In certain embodiments, the crystal is derived from an aqueous solution comprising the α1 chain of α1β1(Cys143-Ala340). In various embodiments, the concentration of α1β1 in the aqueous solution is about 1 to about 50 mg/ml, preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. The precipitating agents used in the invention may be any precipitating agent known in the art, preferably one selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% weight per volume ("w/v") to about 50% w/v, more preferably about 25% w/v. Similarly, the pH of the reservoir solution may be varied, preferably between about 4 to about 10, most preferably about 6.5.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion crystallization is preferred.

Additionally, the claimed invention relates to methods of using the claimed crystal, and the structural coordinates, in methods for screening, designing, or optimizing molecules or other chemical entities that may interfere with the interaction between α1β1

ligands such as members of the extracellular matrix (e.g., collagen) and α1β1. Thus, the structural coordinates of α1β1 or portions thereof can be used to solve the crystal structure of a mutant, homologue or co-complex of α1β1 or a fragment thereof, as well as to solve other unknown crystals which associate with α1β1 or fragments thereof.

In some embodiments, the structural coordinates of the α1 chain of α1β1 (as exemplified in Table II) can be used to evaluate a chemical entity to obtain information about the binding of the chemical entity to α1β1. The structural coordinates can be used to characterize chemical entities which interfere with the relationship between the extracellular matrix (i.e., collagen or laminin) and α1β1 such as inhibitors or agonists. The coordinates can also be used to optimize binding characteristics, to determine the orientation of ligands in a binding site of α1β1. One skilled in the art will appreciate the numerous uses of the claimed invention in the areas of drug design, screening and optimization of drug candidates, as well as in determining additional unknown crystal structures.

In various embodiments, the claimed invention relates to a machine readable data storage medium having a data storage material encoded with machine readable data, which, when read by an appropriate machine, can display a three dimensional representation of a crystal. The crystals displayed comprise a fragment of α1β1 such as that described by the coordinates in Table II, or a crystal having a binding site moiety comprising amino acids Asp154, Ser156, Asn157,Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298.

In other embodiments, the claimed invention relates to a method for determining a at least a portion of a three dimensional structure of a chemical entity or molecular complex by calculating phases from the structural coordinates of a crystal of a fragment of α1β1, calculating the electron density map from the phases obtained, and then determining at least a portion of the unknown structure based upon the electron density map.

In yet other embodiments, the invention relates to methods for evaluating the ability of a chemical entity to associate with α1β1. The methods employ computational or experimental means to perform a fitting operation between the chemical entity and the α1β1 to obtain data related to the association, and analyzing the data to determine the characteristics. Chemical entities identified by these methods which are capable of interfering with the in vivo or in vitro association between the extracellular matrix and

α1β1 are also encompassed by the claimed invention. The claimed chemical entities may comprise binding sites substantially similar to those of α1β1, or, alternatively may comprise binding sites capable of associating with the binding sites of α1β1.

It is to be understood that both the foregoing general description and the following detailed description are exemplary and explanatory and are intended to provide further explanation of the invention as claimed.

The accompanying drawings are included to provide a further understanding of the invention and are incorporated in and constitute a part of this specification, illustrate several embodiments of the invention, and together with the description, serve to explain the principles of the invention.

BRIEF DESCRIPTION OF THE FIGURES

Figure 1: 2Fo-Fc electron density map for a representative region of the α1 I-domain crystal structure, contoured at 1Sigma.

Figure 2: Ribbon representation of the fold of the α1 I-domain molecule. The arrow points to the MIDAS binding site.

DETAILED DESCRIPTION OF THE INVENTION

In order that the invention described herein may be more fully understood, the following detailed description is set forth.

The present invention relates to a crystal of a soluble fragment of the extracellular domain of the α1β1 integrin. Specifically, it relates to a crystal of a soluble protein comprising the sequence from Cys143 to Ala340 of the α1 chain of α1β1 integrin ("sα1β1(143-340)"), the structure of sα1β1(143-340) as determined by X-ray crystallography, and the use of the sα1β1(143-340) structure and that of its homologs, mutants and co-complexes to design, identify, characterize, screen and/or optimize candidate inhibitors or agonists of α1β1 activity.

A. DEFINITIONS

The term α1β1 integrin ("VLA-1" or "α1β1" or "α1β1 integrin", used interchangeably) herein refers to a genus of polypeptides which are capable of binding to members of the extracellular matrix proteins such as laminin or collagen, or homologs or fragments thereof. The term as used herein includes sα1β1 integrin 143-340), homologs, mutants, equivalents and fragments thereof.

The term "co-complex" refers to an α1β1 or a mutant or homolog of α1β1 in covalent or non-covalent association with a chemical entity.

The term "homolog" or "homologous"- as used herein is synonymous with the term "identity" and refers to the sequence similarity between two polypeptides, molecules or between two nucleic acids. When a position in both of the two compared sequences is occupied by the same base or amino acid monomer subunit (for instance, if a position in each of the two DNA molecules is occupied by adenine, or a position in each of two polypeptides is occupied by a lysine), then the respective molecules are homologous at that position. The percentage homology between two sequences is a function of the number of matching or homologous positions shared by the two sequences divided by the number of positions compared x 100. For instance, if 6 of 10 of the positions in two sequences are matched or are homologous, then the two sequences are 60% homologous. By way of example, the DNA sequences CTGACT and CAGGTT share 50% homology (3 of the 6 total positions are matched). Generally, a comparison is made when two sequences are aligned to give maximum homology. Such alignment can be provided using, for instance, the method of Needleman et al., *J. Mol Biol.* 48: 443-453 (1970), implemented conveniently by computer programs such as the Align program (DNAstar, Inc.). Homologous sequences share identical or similar amino acid residues, where similar residues are conservative substitutions for, or "allowed point mutations" of, corresponding amino acid residues in an aligned reference sequence. In this regard, a "conservative substitution" of a residue in a reference sequence are those substitutions that are physically or functionally similar to the corresponding reference residues, e.g., that have a similar size, shape, electric charge, chemical properties, including the ability to form covalent or hydrogen bonds, or the like. Particularly preferred conservative substitutions are those fulfilling the criteria defined for an "accepted point mutation" in Dayhoff et al., 5: **Atlas of Protein Sequence and Structure,** 5: Suppl. 3, chapter 22: 354-352, Nat. Biomed. Res. Foundation, Washington, D.C. (1978).

The term "mutant" refers to an α1β1 integrin or fragment thereof, characterized by the replacement, deletion, or insertion of at least one amino acid from the wild-type. Such a mutant may be prepared, for example, by expression of α1β1 integrin previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

The term " positively charged amino acid" includes any amino acid, natural or unnatural, having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any amino acid, natural or unnatural, having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to $\alpha 1\beta 1$ integrin. The change in surface charge can be determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the pI of the wild-type molecule.

The term "associating with" refers to a condition of proximity between two chemical entities, or portions thereof, for example, an $\alpha 1\beta 1$ integrin or portions thereof and a chemical entity. The association may be non-covalent, wherein the juxtaposition is energetically favored by hydrogen bonding, van der Waals interaction, or electrostatic interaction, or it may be a covalent association.

The term "binding site" refers to any or all of the sites where a chemical entity binds or associates with another entity.

The term "structural coordinates" refers to the coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating units of the crystal. Those skilled in the art will understand that the data obtained are dependent upon the particular system used, and hence, different coordinates may in fact describe the same

crystal if such coordinates define substantially the same relationship as those described herein. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structural coordinates determined by X-ray crystallography is not without standard error. Table II is the atomic coordinates of the I-domain of the α1 chain of α1β1 integrin (143-340). For the purpose of this invention, any set of structural coordinates of α1β1 (143-340) that have a root mean square deviation of equivalent protein backbone atoms of less than about 2Å when superimposed-- using backbone atoms-- on the structural coordinates in Table II shall be considered identical. Preferably the deviation is less than about 1Å and more preferably less than about 0.5Å.

The term "heavy atom derivatization" refers to a method of producing a chemically modified form of a crystallized α1β1 integrin. In practice, a crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which can diffuse through the crystal and bind to the surface of the protein. The location of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information can be used to generate the phase information used to construct the three-dimensional structure of the molecule.

The term "unit cell" refers to a basic shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary structural model of a crystal whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known e.g. the α1 I-domain coordinates in Table II, within the unit cell of the unknown crystal, so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model, and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final accurate

structure of the unknown crystal. See, e.g., Lattman, E., "Use of the Rotation and Translation Functions", Methods in Enzymology, 115, pp. 55-77 (1985); Rossman, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser. No. 13, Gordon and Breach, New York (1972), all specifically incorporated by reference herein. Using the structural coordinates provided by this invention, molecular replacement may be used to determine the structural coordinates of a crystalline co-complex, unknown ligand, mutant, homolog, or of a different crystalline form of α1β1 or fragment thereof. Additionally, the claimed crystal and its coordinates may be used to determine the structural coordinates of a chemical entity which associates with α1β1 or fragment or with a member of the extracellular matrix which is a ligand for α1β1 or fragment thereof.

The term "chemical entity" as used herein shall mean, for example, any molecule, molecular complex, compound or fragment thereof.

Mutants of α1β1 or fragments thereof may be generated by site-specific incorporation of natural or unnatural amino acids into α1β1 or fragments using general biosynthetic methods known to those skilled in the art. For example, the codon encoding the amino acid of interest in wild-type α1 chain of α1β1 may be replaced by a "blank" nonsense codon, such as TAG, using oligonucleotide-directed mutagenesis. A suppressor tRNA directed against this codon can then be chemically aminoacylated in vitro with the desired amino acid. The aminoacylated tRNA can then be added to an in vitro translation system to yield a mutant α1β1 with the site-specific incorporated amino acid.

The term "soluble fragment" of α1β1 and any equivalent term used herein, refers to a functional fragment of α1β1, and more particularly refers to a functional α1 chain. The term "functional" as used in this context refers to a soluble fragment of the extracellular domain that is capable of binding to, or associating with a member of the extracellular matrix such as collagen or laminin or any fragments or homologs thereof, including molecular complexes comprising fragments thereof. Such binding may be demonstrated through immunoprecipitation experiments, using standard protocols known in the art.

A. ALPHA 1 BETA 1 INTEGRIN, its Crystal, and its Biological Implications

It will be understood that throughout the specification and claims, the positional location of the amino acids described is not an absolute value, but rather, defines the relative relationship of the residues. Thus it is intended that the present invention encompass the sequences having the same or similar relative positions.

For the first time, the present invention permits the use of molecular design techniques to design, screen and optimize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of α1β1, in whole or in part. The α1β1 integrin is a membrane-bound protein of considerable biomedical interest because of its involvement in important functions mediated by its binding to the extracellular matrix such as collagen. Since α1β1 is found in various vertebrate (e.g., mammalian) organisms, such as humans, mice, rats, and pigs, the claimed invention is not intended to be limited to any particular species or organism.

The α1β1 integrin (VLA-1)is a member of the integrin family of proteins. The crystal structure of I-domains from other members of this family, αM, αL and α2, have been described. See Dickeson & Santoro (1998) Cell. Mol. Life Sci. 54, 556-566 for a review and Emsley et al., J. Biol.Chem. 272, 28512-28517.

These I-domains were used as a framework for understanding the sα1β1 integrin(143-340) crystal structure. However, despite certain similarities, the differences between the I-domain of α1 and the I-domains of αM, αL, and α2 integrins, confirm that these ligand-receptor systems utilize spatially overlapping, but nonidentical and nonconserved sites of contact residues with different molecular determinants of binding.

Considering the complexity and overlap of the various integrins and their biological processes, the fact that α1β1 binds specifically to its ligand suggests that inhibiting α1β1 signaling may have important therapeutic applications. The crystal structure of sα1β1 (143-340) presented here is expected to be useful in the design, identification, characterization and optimization of such therapeutic agents.

The following detailed description of applicants invention encompasses the (a) crystal structure of the α1 chain I-domain (Cys143-Ala340) of α1β1 integrin and the coordinates thereof, (b) the binding sites thereof, (c) methods of making an α1β1 crystal or fragment thereof, and (d) methods of using the α1β1 crystal or fragment thereof and its structural coordinates.

(a) Crystal Structure of the α1 I-domain

The claimed invention provides crystals of α1β1 integrin as well as the structure derived therefrom. The crystals are derived from the α1 I-domain of the rat. Nevertheless, the sequence identity between rat and human alpha 1 I-domains is about 95%. Specifically, the amino acids which differ between the rat and human α1 I-domains are

Ile166, Asn214, Gly217, Arg 218, Gln219 Leu222, Tyr262, Gln267, His288, Ala330 (rat I-domain sequence). Most of them are located a relatively long distance away from the metal-ion-dependent-adhesion-site (MIDAS) of the α1 I-domain, the site likely to be involved in ligand binding. The only 2 amino acids that are expected to participate in ligand binding are the Leu222 and His288. This high degree of primary amino acid sequence identity indicates that the 3-dimensional structures of rat and human 1 I-domains are expected to be similar. Therefore, we used the crystal structure of the rat 1 I-domain for the purposes discussed in this patent and we fully expect that the 3-dimensional structure of the human 1 I-domain will have substantially identical coordinates for the main chain atoms.

The claimed invention provides crystals of a fragment from the α1 chain of α1β1 integrin(143-340) having unit cells which are rhombohedral, and having the following dimensions a= 34.77Å ; b=85.92Å and c= 132.56Å; α=β= γ= 90Å. Almost all of the residues of the I-domain of the α1 chain of α1β1 integrin, except for residues 143-144 of the N terminus and 336-340 of the C-terminus, are well defined in the final electron density map shown in Figure 1. The current model consists of 386 amino acid residues and 199 water molecules with a crystallographic R factor of 23.5 % and an R_{free} of 30.2% for data between 100Å and 2.2Å.

There are two copies of the molecule (termed "A" and "B") in the asymmetric unit. The Ramachandran diagram shows that 384 out of the 386 amino acid residues have (φ,ψ) angles within the allowed regions. The exception is residue Glu192 (A & B). In the atomic coordinates of the rat I-domain crystal structure (Tabld II), residues Thr145, Gln146, Arg234 of molecule A and Thr145 and Arg175 of molecule B are modeled as alanines because of absence of electron density for the side chain. In addition, residues 143, 145, 337, 338, 339,340 of molecule A and 143, 144, 339, 340 of molecule B are not included in the model due to weak electron density.

The I-domain adopts the nucleotide-binding fold (Figure 2) characterized by the existence of seven helices surrounding a core of five parallel β-strands and one antiparallel β-strand. The dimensions of the molecule are 25Å x 30Å x 50Å. The overall fold is similar to that of αM, αL and α2 I-domains and in particular to that of the α2 I-domain. By homology to the other I-domains it is inferred that the metal-ion-dependent-adhesion-site (MIDAS) of the α1 I-domain consists of residues Asp154, Ser156, Ser158, Thr224, Asp

257. The MIDAS site is the site of Mg or Mn cation binding and is expected to be involved in ligand binding. The crystals were grown in the absence of Mg or Mn cations (except for contaminants) and there is no electron density visible in that would correspond to a cation. The structure appears to have the "inactive" conformation according to the model proposed in Lee et al. (1995) Structure 3, 1333-1340. The conformations of molecules A and B are very similar.

(b) Binding Sites

Modeling studies done for collagen binding on the α2 I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) suggest that the binding site for collagen is expected to include the MIDAS site as well as several neighboring residues. By analogy, the binding site of the α1 I-domain for collagen is expected to include residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. Of interest is the observation that the MIDAS site of the α1 I-domain (molecule A in the crystal) forms an interaction with Arg246 of molecule B. It is possible that the positive charge of the arginine side chain replaces the positive charge of the missing metal ion.

(c) Methods of Making an α1β1 Crystal

In various embodiments, the claimed invention relates to methods of preparing crystalline forms of α1β1, or fragments thereof by first providing an aqueous solution comprising α1β1 or a fragment of α1β1. A reservoir solution comprising a precipitating agent is then mixed with a volume of the α1β1 solution and the resultant mixed volume is then crystallized. In certain embodiments, the crystal is derived from an aqueous solution comprising sα1β1(127-340). In preferred embodiments, the crystal is derived from an aqueous solution comprising sα1β1(143-340). The concentration of α1β1 or fragment in the aqueous solution may vary, and is preferably about 1 to about 50 mg/ml, more preferably about 5 mg/ml to about 15 mg/ml, and most preferably, about 10 mg/ml. Similarly, precipitating agents used in the invention may vary, and may be selected from any precipitating agent known in the art. Preferably the precipitating agent is selected from the group consisting of sodium citrate, ammonium sulfate and polyethylene glycol, with polyethylene glycol 8000 being most preferred. Any concentration of precipitating agent may be used in the reservoir solution, however it is preferred that the concentration be about 20% w/v to about 35%w/v, more preferably about 25% w/v. The pH of the

reservoir solution may also be varied, preferably between about 4 to about 10, most preferably about 6.5. One skilled in the art will understand that each of these parameters can be varied without undue experimentation and acceptable crystals will still be obtained. In practice, once the appropriate precipitating agents, buffers or other experimental variables are determined for any given growth method, any of these methods or any other methods can be used to grow the claimed crystals. One skilled in the art can determine the variables depending upon his particular needs.

Various methods of crystallization can be used in the claimed invention, including, but not limited to, vapor diffusion, batch, liquid bridge, or dialysis. Vapor diffusion crystallization is preferred. See, e.g. McPherson et al., "Preparation and Analysis of Protein Crystals", Glick,. Ed., pp 82-159, John Wiley & Co. (1982); Jancarik et.al., "Sparse matrix sampling: a screening method for crystallization of protein", J. Appl. Cryst. 24, 409-411 (1991), specifically incorporated by reference herein.

In vapor diffusion crystallization, a small volume (i.e. a few milliliters) of protein solution is mixed with a solution containing a precipitating agent. This mixed volume is suspended over a well containing a small amount, i.e. about 1 ml, of precipitating solution. Vapor diffusion from the drop to the well will result in crystal formation in the drop.

The dialysis method of crystallization utilizes a semipermeable size exclusion membrane which retains the protein but allows small molecules (i.e. buffers and precipitating agents) to diffuse in and out. In dialysis, rather than concentrating the protein and the precipitating agent by evaporation, the precipitating agent is allowed to slowly diffuse through the membrane and reduce the solubility of the protein while keeping the protein concentration fixed.

The batch methods generally involve the slow addition of a precipitating agent to an aqueous solution of protein until the solution just becomes turbid, at this point the container can be sealed and left undisturbed for a period of time until crystallization occurs.

Thus, applicants intend that the claimed invention encompass any and all methods of crystallization. One skilled in the art can choose any of such methods and vary the parameters such that the chosen method results in the desired crystals.

(d) Use of ALPHA 1 BETA 1 INTEGRIN Crystal and its Coordinates

The claimed crystals, and coordinates describing them, permit the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds or agonists capable of binding to, or associating with, the binding site of α1β1 integrin in whole or in part.

One approach enabled by this invention is the use of the structural coordinates defined herein to design chemical entities that bind to or associate with, α1β1 or fragments of α1β1 and alter the physical properties of the compounds in different ways. Thus, properties such as, for example, solubility, affinity, specificity, potency, on/off rates or other binding characteristics may all be altered and/or optimized.

One may design desired chemical entities by probing a crystal of the present invention with a library of different entities to determine optimal sites for interaction between candidate chemical entities and α1β1 or fragments of α1β1. For example, high resolution x-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for the desired activity. Once the desired activity is obtained, the molecules can be further optimized.

The claimed invention also makes it possible to computationally screen small molecule data bases or computationally design chemical entities or compounds that can bind in whole, or in part, to extracellular matrix proteins or α1β1 or fragments thereof. They may also be used to solve the crystal structure of mutants, co-complexes, or of the crystalline form of any other molecule homologous to, or capable of associating with, at least a portion of α1β1, i.e., the I-domain of the α1 chain.

One method that may be employed for this purpose is molecular replacement. An unknown crystal structure, which may be any unknown structure, such as, for example, another crystal form of α1β1, an α1β1 mutant, or a co-complex with an extracellular matrix protein such as laminin or collagen, or any other unknown crystal of a chemical entity which associates with α1β1 or fragment which is of interest, may be determined using the structural coordinates of this invention, set forth in Table II. Co-complexes with α1β1 or fragments may include, but are not limited to, laminin-α1β1, collagen-α1β1, and "small molecule"-α1β1. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information without the claimed invention. The information obtained can thus be used to

optimize potential inhibitors or agonists of α1β1, and more importantly, to design and synthesize novel classes of chemical entities which will affect the relationship between α1β1 and its ligand(s) in the extracellular matrix.

The design of compounds that inhibit or agonize α1β1 according to this invention generally involves consideration of at least two factors. First, the compound must be capable of physically or structurally associating with α1β1 or a fragment thereof. The association may be any physical, structural, or chemical association, such as, for example, covalent or noncovalent bonding, van der Waals interactions, hydrophobic or electrostatic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with α1β1 or fragment thereof. Although not all portions of the compound will necessarily participate in the association with α1β1 or fragment, those non-participating portions may still influence the overall conformation of the molecule. This in turn may have a significant impact on the desirability of the compound. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site.

The potential inhibitory or binding effect of a chemical compound on α1β1 or fragment may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and α1β1 or its fragment(s), the need for synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to α1β1 or fragment thereof. Thus, expensive and time consuming synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of α1β1 or fragment may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites of α1β1.

Thus, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with α1β1 and more particularly, with the individual binding sites of the I-domain of the α1 chain of α1β1(143-340). This process may begin by visual inspection of, for example, the binding site on a computer screen

based on the coordinates in Table II. Selected fragments or chemical entities may then be positioned in a variety of orientations, or "docked", within an individual binding pocket of α1β1. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may be of use for selecting interesting fragments or chemical entities. (GRID, available from Oxford University, Oxford, UK; MCSS or CATALYST, available from Molecular Simulations, Burlington, MA; AUTODOCK, available from Scripps Research Institute, La Jolla, CA; DOCK available from University of California, San Francisco, CA., XSITE, University College of London, UK.)

Once suitable chemical entities or fragments have been selected, they can be assembled into an inhibitor or agonist. Assembly may be by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen, in relation to the structural coordinates disclosed herein.

Alternatively, one may design the desired chemical entities "de novo", experimentally, using either an empty binding site, or optionally including a portion of a molecule with desired activity. Thus, for example, one may use solid phase screening techniques where either α1β1 or a fragment thereof, or candidate chemical entities to be evaluated are attached to a solid phase thereby identifying potential binders for further study or optimization.

Basically, any molecular modeling techniques may be employed in accordance with the invention; these techniques are known, or readily available to those skilled in the art. It will be understood that the methods and compositions disclosed herein can be used to identify, design or characterize not only entities which will associate or bind to α1β1 or fragment thereof, but alternatively to identify, design or characterize entities which, like α1β1, will bind to extracellular matrix proteins, thereby disrupting the α1β1-ECM interaction. The claimed invention is intended to encompass these methods and compositions broadly.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to α1β1 or fragment thereof may be tested and optimized using computational or experimental evaluation. Various parameters can be optimized depending on the desired result. These include, but are not limited to,

specificity, affinity, on/off rates, hydrophobicity, solubility and other characteristics readily identifiable by the skilled artisan. Thus, one may optionally make substitutions, deletions, or insertions in some of the components of the chemical entities in order to improve or modify the binding properties. Generally, initial substitutions are conservative, i.e the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original component.

The present invention also enables the design of mutants of α1β1 and the solving of their crystal structure. More particularly, the claimed invention enables one skilled in the art to determine the location of binding sites and interfaces, particularly in the I-domain of the α1 chain. thereby identifying desirable sites for mutation.

For example, mutation may be directed to a particular site or combination of sites on the I-domain, by replacing or substituting one or more amino acid residues. Such mutants may have altered binding properties which may or may not be desirable.

The mutants may be prepared by any methods known in the art, such as for example, site directed mutagenesis, deletion or addition, and then tested for any properties of interest. For example, mutants may be screened for an altered charge at a particular pH, tighter binding, better specificity etc.

Additionally, the claimed invention is useful for the optimization of potential small molecule drug candidates. Thus, the claimed crystal structures can be also be used to obtain information about the crystal structures of complexes of the α1β1 integrin and small molecule inhibitors. For example, if the small molecule inhibitor is co-crystallized with α1β1 or a fragment thereof, then the crystal structure of the complex can be solved by molecular replacement using the known coordinates of α1β1 or fragment for the calculation of phases. Such information is useful, for example, for determining the nature of the interaction between the I-domain of α1β1 integrin and the small molecule inhibitor, and thus, may suggest modifications which would improve binding characteristics such as affinity, specificity and kinetics.

Example 1: <u>Determination of Crystal Structure of the ALPHA 1 INTEGRIN I-DOMAIN (127-340)</u>

A. Expression and purification of α1 integrin I-domain.

A soluble fragment of the extracellular domain of rat integrin α1β1 α1 chain containing amino acid residues Val127 to the C-terminal residue Ala340 was produced in

soluble form and purified as follows: The gene encoding the rat α1β1 I-domain sequence of amino acids Val127-Ala340 of the α1 chain was amplified from full length cDNAs by the polymerase chain reaction (PCR) (PCR CORE Kit; Boehringer Mannheim, GmbH Germany), using rat specific primers (5'-CAGGATCCGTCAGTCCTACATTTCAA-3' [forward][SEQ ID NO: 1]; 5'-TCCTCGAGCGCTTCCAAAGCGAATAT-3' [reverse]{SEQ ID NO: 2] .

The resulting PCR amplified products were purified over a PCR select II column (5 prime-3 prime), digested with Bam H1 and Xho 1 restriction enzymes, re-purified over a PCR select II column, and ligated in pGEX4t (Pharmacia), previously digested with Bam H1 and Xho1, dephosphorylated with calf intestinal alkaline phosphatase (New England Biolabs), and gel purified. Ligation products were transformed into competent DH5A E.Coli cells (Gibco BRL) and the resulting amplicillin resistant colonies were screened for the expression of the ~45 kDa glutathione S-transferase-I domain fusion protein. The I-domain was expressed as a GST fusion protein with a thrombin cleavage site at the junction of the sequences.

Cells in PBS (1 part of wet cell weight to 4 parts of buffer) were lysed in a Gaulin press and clarified of particulates by centrifugation (14,000 x g, 30 min). 650 ml of lysate from 180 g of cell paste was loaded onto a 25 ml glutathione Sepharose 4B column (Pharmacia). The column was washed with 100 ml of PBS and the rat alpha1 integrin I domain-GST fusion protein eluted from the column with 50 mM Tris HCl pH 8.0, 5 mM glutathione (reduced). Five ml fractions were collected and analyzed for total protein by absorbance at 280 nm and for purity by SDS-PAGE. Peak fractions were pooled, aliquoted, and stored at –70 degrees C. A total of 375 mg of the fusion protein (15 mg/ml) at >90% purity was recovered.

For preparation of the purified I-domain, 6 ml of the fusion protein was dialyzed overnight against one liter of 50 mM Tris pH 7.5. The sample was treated with 100 µg of thrombin (a gift of Dr. John Fenton, New York State Department of Health, Albany, NY) for 150 min at room temperature. DTT was added to 2 mM and the sample was loaded onto a 7 ml glutathione Sepharose® 4B column. The flow through from the column was collected as 1.5 ml fractions and the column was further washed with 50 mM Tris HCl pH 7.5, 2 mM DTT buffer. The flow through and wash fractions were analyzed for

absorbance at 280 nm. Peak fractions were pooled and loaded onto a 2.4 ml Q Sepharose® FF column (Pharmacia).

The Q-Sepharose column was washed with 2 ml of 50 mM Tris HCl pH 7.5, 2 mM DTT; 2 ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol; twice with 2ml of 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 25 mM NaCl; and the alpha 1 integrin I domain eluted with 50 mM Tris HCl pH 7.5, 10 mM 2-mercaptoethanol, 75 mM NaCl. Peak fractions were pooled, filtered through a 0.2 μm filter, and stored at 4 degrees C. The final product was >99% pure by SDS-PAGE, eluted as a single peak by size exclusion chromatography on a Superose® 6 column (Pharmacia & Upjohn) consistent with its predicted mass, and by electrospray ionization-mass spectrometry (ESI-MS, Micromass, Quattro-II, Manchester, UK) contained a single ion with mass of 24,868 Da, which agreed with the predicted mass of 24871.2 Da for the rat α1 I-domain sequence plus the GS linker resulting from cleavage at the engineered thrombin cleavage site. From 72 mg of the fusion protein, 24 mg of the purified I- domain was recovered (based on a theoretical extinction coefficient of 0.5 at 280 nm for 1 mg/ml solution of the I-domain).

In preliminary studies, we found that the rat α1 integrin I-domain in this form failed to crystallize under any test condition and, as had been observed for other I domains (R.Liddington, personal communication), that sequences at the N-terminus of the I domain construct were problematic. A simple proteolytic method was developed to convert the purified rat I-domain into a form that could be crystallized.

Briefly, 240 μl of the purified alpha 1 integrin I domain (16 mg/ml) was diluted with 360 μl of 50 mM Tris HCl pH 7.5 and loaded onto a 1.2 ml V8 protease column (Pierce) that had been equilibrated in 50 mM Tris HCl pH 7.5. The I domain solution was left in contact with the resin for 35 min at room temperature and then recovered by washing the column with 50 mM Tris HCl pH 7.5. The I domain was then dialyzed overnight against 10 mM Tris pH 7.5, 10 mM 2-mercaptoethanol and concentrated to 11 mg/ml in a centricon-10 ultrafiltration unit (Amicon). ESI-MS analysis of V8 protease digested product revealed that the product had been converted into a des 1-18 form, starting at Cys143 in the fusion protein construct.

B. Crystallization

Buffer chemicals were purchased from Fisher (Boston, MA). Crystallization condition screenings were done with the Crystal Screen I kit from Hampton Research

(Riverside, CA). Crystals were grown by the vapor diffusion method of Jancarik & Kim (1991) J. Appl. Crystallogr. 24, 409-411.

In order to find conditions of crystallization, an incomplete factorial screen was set up. In a typical experiment, protein solution was mixed with an equal volume of reservoir solution and a drop of the mixture was suspended under a glass cover slip over the reservoir solution. Crystals were grown out of 25% w/v Polyethylene Glycol (PEG) 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate reservoir solution. The crystals are shaped as plates, are easy to reproduce and can reach maximum dimensions of almost 0.5 mm on one side. Variation of pH between 6 and 7 did not affect crystal quality.

Those of skill in the art will appreciate that the aforesaid crystallization conditions can be varied. By varying the crystallization conditions, other crystal forms of α1β1 integrin I-domain may be obtained. Such variations may be used alone or in combination, and include: varying final protein concentrations between 5 mg/ml and 35 mg/ml; varying the sα1β1 integrin I-domain to precipitant ratio; varying PEG concentrations between 15% and 35% w/v; varying the molecular weight of polyethylene glycol from 400 to 8000; varying pH ranges between 5.0 and 9.5; varying sodium cacodylate concentrations between 5 and 395 mM; varying sodium acetate concentrations between 5 and 495 mM; varying the concentration or type of detergent; varying the temperature between -5 degrees C and 30 degrees C; and crystallizing α1β1 integrin I-domain by batch, liquid bridge, or dialysis method using the above conditions or variations thereof. See McPherson, A.(1982). Preparation and Analysis of Protein Crystals. (Glick, ed.) pp. 82-159, John Wiley & Co., N.Y., specifically incorporated by reference herein.

C. Data collection and processing

Crystals were equilibrated gradually in a cryoprotectant solution of 20% glycerol, 25% w/v PEG 8000, 0.1 M sodium cacodylate pH 6.5, 0.2 M sodium acetate, and were mounted on a loop and immediately frozen in a -150 C liquid nitrogen gas stream. The technique of freezing the crystals essentially immortalizes them and produced a much higher quality data set.

A native X-ray data set up to 3.0 Å resolution was collected from one crystal by using an R-AXIS II image plate detector system (Molecular Structure Corporation, Woodlands, TX). A second data set to 2.2 Å resolution was collected later by using a

larger crystal. The data were integrated and reduced using the HKL program package (Otwinowski et al (1993) in Data collection and Processing pp 80-86, SERC Daresbury Laboratory, Warrington, UK). The data collection required about 4 days. Data processing suggested an orthorhombic unit cell with approximate cell dimensions a=34.77 Å , b=85.92 c=132.56 and alpha=beta=gamma=90. The space group was identified as $P2_12_12_1$. The 2.2 Å data set was 91.3% complete and had an R-merge of 5.6%. Calculation of the Matthews volume gives $V_M = 4.22$ assuming a molecular weight of 23,000 daltons which suggested that there are 2 molecules in the asymmetric unit.

D. Molecular replacement

All subsequent molecular replacement computing was done with the program Amore (Navaja et al (1994) Acta Crystallogr. A 50, 157-163) from the CCP4 program package (The SERC (UK) Collaborative Computing Project No 4, Daresbury Laboratory, UK 1979). Molecular graphics manipulations were done with QUANTA (Molecular Simulations, Inc.) and "O" software (Jones et al 1991 Acta Crystallogr. A 47, 110-119). The coordinates of the crystal structure of the human α2 I-domain (Emsley et al. (1997) J. Biol.Chem. 272, 28512-28517) was used as a probe for rotation and translation searches using the 3 Å data set.

We used all the coordinates of all atoms, including side chains. The rotation function gave a solution with the highest correlation coefficient (cc) of 9.7. This solution was used for a first translation function which yielded a cc of 24.6 and an R-factor of 48.7%. Using rigid body refinement, these values refined to cc=40.3, R-factor=48.7%. Using this first solution, we took the peaks of the first rotation search and used these for searching the second molecule, keeping our first solution fixed. The translation search yielded a maximum peak with cc=37.3 and an R-factor of 44.8%. Rigid body refinement on these two solutions resulted in cc=56.3 and R-factor=43.3%.

The next highest solution gave: cc=36.6 R-fac=49.9%. By generating symmetry related molecules and displaying them with computer graphics it was found that they packed satisfactorily in the unit. The rotation matrix between the two molecules of the asymmetric unit was determined and one molecule was used for the initial stages of model building.

E. Model building and crystallographic refinement

All subsequent refinement computing was done with the XPLOR program (Brunger et al (1987) Science 235, 458-460). 10% of the data were used for the calculation of R-free. To reduce model bias, partial models were used for map calculation and refinement. The initial partial model, containing a polyalanine chain of the secondary structure elements only, from the a2 I-domain structure, was subjected to conventional positional refinement and grouped B-factor refinement with strict non -crystallographic symmetry constraints.

The R and R-free factors dropped to 32.3% and 39.4% respectively. 3Fo -2Fc maps were used for cycles of model building and refinement. The resolution range used was from 8 to 3 Å. Typically, cycles consisted of model building, positional refinement and B-factor refinement. When the R and R-free reached 26% and 36% respectively, the 3 Å data set did not allow further improvement of the model. The 2.2 Å data set was collected at this point and was used for all subsequent model building and refinement. The R and R-free factors after the initial rigid body refinement at 2.2 Å were 41.3% and 42.2% respectively.

This larger data set allowed use of simulated annealing refinement and torsion angle dynamics refinement. As the phases improved, more atoms were added into the model. Initially, grouped B-factors were assigned for each residue (one for main chain and the one for side chain atoms). Later, non-crystallographic symmetry constraints were removed and individual atomic B-factors where refined for each residue. In addition bulk solvent correction was applied to the data set. Residues and side chains would be incorporated in the model if they were sufficiently well defined in 3Fo-2Fc electron density maps. Only manual structure modifications that resulted in lower R-free after refinement were accepted.

When R and R-free reached 29% and 34.8% respectively, water molecules were added by using the X-solvate utility of QUANTA. Finally, maximum likelihood refinement was used (Adams et al (1997) Pro.Nat.Acad.Sci USA 94, pp. 5018-5023) and resulted in the final structure with R and R-free of 23.5% and 30.2% respectively for data between 100 and 2.2 Å resolution. Table I summarizes information regarding crystallographic data and refinement. Table II lists the atomic coordinates of the I-domain of the $\alpha 1$ chain of the rat $\alpha 1\beta 1$ integrin. The coordinates of the crystal structure of the I-

domain may be used in the structure-based design of small molecule inhibitors of α1β1, computational drug design and iterative structure optimization.

a. Computational drug design

Small molecule inhibitors can be designed using computational approaches. These approaches are also known as de novo drug design. In brief, the crystal structure coordinates of the α1β1 integrin or fragment(s) thereof are the input for a computer program, such as DOCK. Programs such as DOCK output a list of small molecule structures that are expected to bind to α1β1 or the fragment(s). These molecules can then be screened by biochemical assays for α1β1 binding. Typically, biochemical assays that screen molecules for their ability to bind to α1β1 or a fragment thereof are competition-type assays. In such assays, the molecule is added to the assay solution and the degree of inhibition is measured using conventional methodology.

An example of such an assay is the following: 96 well plates can be coated with collagen IV or collagen I and blocked with 3% Bovine Serum Albumin solution. Solution of a1 I-domain together with the small molecule under testing are incubated on the coated plates at room temperature for 1 hour and washed in triton buffer. Bound a1 I-domain is detected with a biotinylated anti-I-domain antibody. Plates are read at OD_{405} on a microplate reader. The amount of bound I-domain is compared with a control experiment with no small molecule present. If it is lower than that of the control experiment that suggests inhibition by the small molecule.

b. Iterative cycles of structure optimization

The crystal structures of complexes formed between α1β1 or a fragment and small molecule inhibitors may be solved. In brief, small molecule inhibitors are typically found using the crystal structure coordinates of a sα1β1 integrin or fragment either by the computational approaches mentioned above or by the screening of small molecule libraries. The small molecule inhibitor is then co-crystallized with α1β1 or a fragment and the crystal structure of the complex is solved by molecular replacement. Molecular replacement requires the coordinates of a sα1β1 or fragment for the calculation of phases. The information collected from these experiments can be used to optimize the structure of small molecule inhibitors by clarifying how small molecules interact with the protein target. This suggests ways of modifying the small molecule to improve its

physicochemical properties, such as affinity, specificity, and kinetics with regard to the α1β1 target.

In addition to being necessary for computational drug design and structure optimization, the crystal coordinates described herein are useful for analyzing the α1β1 binding site. Through such analysis, it was determined that a particularly attractive region for drug targeting is in the vicinity of residues Asp154, Ser156, Asn157, Ser158, Leu222, Gln223, Thr224, Asp257, Glu259, His261, His288, Tyr289, Gly292, Leu294 and Lys298. The above observations and hypotheses suggest that this region may contribute significantly to the binding energy of α1β1/ECM interactions, and therefore, is an attractive target for inhibitor design. Site mutations studies can be used in conjunction with the above-described processes to further define the binding site.

It will be apparent to those skilled in the art that various modifications and variations can be made in the methods and compositions of the present invention without departing from the spirit or scope of the invention. Thus, it is intended that the present invention cover the modifications and variations of this invention provided that they come within the scope of the appended claims and their equivalents.

TABLE I: Crystallographic data statistics:

Symmetry:	$P2_12_12_1$
Unit cell (Å)	a = 34.77, b = 85.92, c = 132.56
No.of crystals: 1	
Resolution (Å)	2.2
Reflections(unique):	19,238
R_{merge}	5.6%
Completeness:	91.3%
Completeness(2.2-2.28 Å) 77.6%	

TABLE II: Crystallographic coordinates of the alpha1 I-domain crystal structure in PDB(XPLOR) format. Segment names A, B, W correspond to molecule A, molecule B and water respectively.

```
CRYST    34.770   85.920  132.560  90.00  90.00   90.00  P212121
ATOM      1  CB  ALA   145      35.261  87.828 -14.480  1.00 46.82      A
ATOM      2  C   ALA   145      33.051  87.078 -15.373  1.00 48.98      A
ATOM      3  O   ALA   145      32.414  87.150 -14.310  1.00 49.22      A
ATOM      4  HT1 ALA   145      33.390  89.717 -14.876  1.00  0.00      A
ATOM      5  HT2 ALA   145      33.206  89.509 -16.551  1.00  0.00      A
ATOM      6  N   ALA   145      33.860  89.407 -15.751  1.00 47.03      A
ATOM      7  HT3 ALA   145      34.705  89.992 -15.916  1.00  0.00      A
ATOM      8  CA  ALA   145      34.266  87.977 -15.619  1.00 46.67      A
```

	ATOM	9	N	ALA	146	32.737	86.234	-16.358	1.00	42.12	A
	ATOM	10	H	ALA	146	33.287	86.229	-17.170	1.00	0.00	A
	ATOM	11	CA	ALA	146	31.603	85.321	-16.264	1.00	40.10	A
	ATOM	12	CB	ALA	146	31.657	84.314	-17.389	1.00	35.92	A
	ATOM	13	C	ALA	146	31.621	84.602	-14.919	1.00	40.80	A
	ATOM	14	O	ALA	146	32.511	83.799	-14.647	1.00	42.91	A
	ATOM	15	N	LEU	147	30.629	84.888	-14.082	1.00	37.99	A
	ATOM	16	H	LEU	147	29.931	85.517	-14.359	1.00	0.00	A
	ATOM	17	CA	LEU	147	30.562	84.284	-12.759	1.00	37.93	A
	ATOM	18	CB	LEU	147	31.411	85.107	-11.803	1.00	38.26	A
	ATOM	19	CG	LEU	147	31.994	84.349	-10.623	1.00	39.33	A
	ATOM	20	CD1	LEU	147	33.183	83.510	-11.078	1.00	33.15	A
	ATOM	21	CD2	LEU	147	32.389	85.347	-9.567	1.00	38.31	A
	ATOM	22	C	LEU	147	29.156	84.164	-12.181	1.00	36.60	A
	ATOM	23	O	LEU	147	28.417	85.142	-12.132	1.00	37.06	A
	ATOM	24	N	ASP	148	28.780	82.966	-11.751	1.00	36.31	A
	ATOM	25	H	ASP	148	29.384	82.200	-11.844	1.00	0.00	A
	ATOM	26	CA	ASP	148	27.468	82.788	-11.140	1.00	33.40	A
	ATOM	27	CB	ASP	148	26.836	81.461	-11.589	1.00	35.41	A
	ATOM	28	CG	ASP	148	26.085	81.583	-12.925	1.00	33.40	A
	ATOM	29	OD1	ASP	148	25.783	80.537	-13.531	1.00	32.84	A
	ATOM	30	OD2	ASP	148	25.795	82.715	-13.376	1.00	33.54	A
	ATOM	31	C	ASP	148	27.695	82.829	-9.622	1.00	28.37	A
	ATOM	32	O	ASP	148	28.475	82.050	-9.070	1.00	26.95	A
	ATOM	33	N	ILE	149	27.027	83.767	-8.961	1.00	25.21	A
	ATOM	34	H	ILE	149	26.411	84.349	-9.453	1.00	0.00	A
	ATOM	35	CA	ILE	149	27.179	83.957	-7.529	1.00	24.78	A
	ATOM	36	CB	ILE	149	27.883	85.308	-7.229	1.00	25.55	A
	ATOM	37	CG2	ILE	149	28.047	85.509	-5.718	1.00	19.80	A
	ATOM	38	CG1	ILE	149	29.233	85.363	-7.947	1.00	21.46	A
	ATOM	39	CD1	ILE	149	29.730	86.775	-8.168	1.00	25.74	A
	ATOM	40	C	ILE	149	25.853	83.957	-6.786	1.00	27.12	A
	ATOM	41	O	ILE	149	24.957	84.737	-7.097	1.00	27.87	A
	ATOM	42	N	VAL	150	25.748	83.101	-5.780	1.00	29.44	A
	ATOM	43	H	VAL	150	26.498	82.509	-5.564	1.00	0.00	A
	ATOM	44	CA	VAL	150	24.525	83.031	-4.990	1.00	31.56	A
	ATOM	45	CB	VAL	150	23.914	81.612	-5.015	1.00	33.68	A
	ATOM	46	CG1	VAL	150	22.921	81.433	-3.871	1.00	36.22	A
	ATOM	47	CG2	VAL	150	23.218	81.387	-6.339	1.00	35.65	A
	ATOM	48	C	VAL	150	24.751	83.443	-3.543	1.00	29.32	A
	ATOM	49	O	VAL	150	25.643	82.939	-2.849	1.00	27.25	A
	ATOM	50	N	ILE	151	23.936	84.383	-3.096	1.00	29.18	A
	ATOM	51	H	ILE	151	23.269	84.772	-3.699	1.00	0.00	A
	ATOM	52	CA	ILE	151	24.016	84.847	-1.724	1.00	28.46	A
	ATOM	53	CB	ILE	151	23.614	86.340	-1.625	1.00	27.62	A
	ATOM	54	CG2	ILE	151	23.843	86.860	-0.209	1.00	24.70	A
	ATOM	55	CG1	ILE	151	24.457	87.167	-2.607	1.00	27.55	A
	ATOM	56	CD1	ILE	151	23.788	87.443	-3.933	1.00	28.07	A
	ATOM	57	C	ILE	151	23.067	83.964	-0.908	1.00	26.00	A
	ATOM	58	O	ILE	151	21.923	83.721	-1.307	1.00	25.72	A
	ATOM	59	N	VAL	152	23.575	83.445	0.199	1.00	22.21	A
	ATOM	60	H	VAL	152	24.506	83.650	0.427	1.00	0.00	A
	ATOM	61	CA	VAL	152	22.813	82.581	1.099	1.00	23.05	A
	ATOM	62	CB	VAL	152	23.585	81.247	1.402	1.00	26.59	A
	ATOM	63	CG1	VAL	152	22.665	80.246	2.127	1.00	25.59	A
	ATOM	64	CG2	VAL	152	24.102	80.628	0.094	1.00	21.54	A
	ATOM	65	C	VAL	152	22.689	83.412	2.366	1.00	20.44	A
	ATOM	66	O	VAL	152	23.554	83.369	3.246	1.00	14.87	A
	ATOM	67	N	LEU	153	21.613	84.180	2.442	1.00	20.46	A
	ATOM	68	H	LEU	153	20.950	84.144	1.721	1.00	0.00	A
	ATOM	69	CA	LEU	153	21.384	85.071	3.563	1.00	19.62	A
	ATOM	70	CB	LEU	153	20.780	86.370	3.044	1.00	27.82	A
	ATOM	71	CG	LEU	153	20.357	87.482	4.001	1.00	29.39	A
	ATOM	72	CD1	LEU	153	21.555	88.057	4.739	1.00	32.60	A
	ATOM	73	CD2	LEU	153	19.683	88.565	3.170	1.00	34.32	A
	ATOM	74	C	LEU	153	20.518	84.490	4.659	1.00	22.92	A
	ATOM	75	O	LEU	153	19.360	84.122	4.445	1.00	20.87	A
	ATOM	76	N	ASP	154	21.101	84.430	5.846	1.00	20.52	A
	ATOM	77	H	ASP	154	22.026	84.747	5.930	1.00	0.00	A
	ATOM	78	CA	ASP	154	20.439	83.917	7.020	1.00	20.46	A
	ATOM	79	CB	ASP	154	21.506	83.624	8.078	1.00	22.44	A
	ATOM	80	CG	ASP	154	20.946	83.418	9.462	1.00	20.33	A
	ATOM	81	OD1	ASP	154	19.773	83.017	9.617	1.00	25.28	A

ATOM	82	OD2	ASP	154	21.709	83.658	10.408	1.00	17.38	A
ATOM	83	C	ASP	154	19.463	85.012	7.445	1.00	24.81	A
ATOM	84	O	ASP	154	19.850	86.170	7.680	1.00	19.94	A
ATOM	85	N	GLY	155	18.186	84.645	7.491	1.00	22.66	A
ATOM	86	H	GLY	155	17.945	83.724	7.270	1.00	0.00	A
ATOM	87	CA	GLY	155	17.154	85.583	7.865	1.00	25.80	A
ATOM	88	C	GLY	155	16.573	85.333	9.242	1.00	27.90	A
ATOM	89	O	GLY	155	15.411	85.623	9.465	1.00	30.07	A
ATOM	90	N	SER	156	17.363	84.783	10.158	1.00	29.73	A
ATOM	91	H	SER	156	18.280	84.539	9.917	1.00	0.00	A
ATOM	92	CA	SER	156	16.887	84.533	11.519	1.00	33.03	A
ATOM	93	CB	SER	156	17.956	83.778	12.327	1.00	33.06	A
ATOM	94	OG	SER	156	18.696	84.658	13.163	1.00	34.46	A
ATOM	95	HG	SER	156	19.354	84.158	13.652	1.00	0.00	A
ATOM	96	C	SER	156	16.589	85.896	12.162	1.00	28.30	A
ATOM	97	O	SER	156	16.928	86.935	11.595	1.00	32.92	A
ATOM	98	N	ASN	157	15.958	85.892	13.335	1.00	27.00	A
ATOM	99	H	ASN	157	15.732	85.033	13.746	1.00	0.00	A
ATOM	100	CA	ASN	157	15.591	87.140	14.032	1.00	22.66	A
ATOM	101	CB	ASN	157	14.545	86.871	15.127	1.00	24.65	A
ATOM	102	CG	ASN	157	13.322	86.095	14.644	1.00	26.95	A
ATOM	103	OD1	ASN	157	12.722	85.354	15.422	1.00	22.76	A
ATOM	104	ND2	ASN	157	12.941	86.269	13.380	1.00	23.43	A
ATOM	105	HD21	ASN	157	13.442	86.879	12.800	1.00	0.00	A
ATOM	106	HD22	ASN	157	12.156	85.772	13.074	1.00	0.00	A
ATOM	107	C	ASN	157	16.724	87.922	14.717	1.00	20.73	A
ATOM	108	O	ASN	157	16.488	89.024	15.179	1.00	19.35	A
ATOM	109	N	SER	158	17.936	87.382	14.804	1.00	20.15	A
ATOM	110	H	SER	158	18.117	86.511	14.395	1.00	0.00	A
ATOM	111	CA	SER	158	19.005	88.099	15.519	1.00	17.25	A
ATOM	112	CB	SER	158	20.003	87.095	16.115	1.00	18.79	A
ATOM	113	OG	SER	158	20.309	86.048	15.204	1.00	21.49	A
ATOM	114	HG	SER	158	20.692	86.418	14.407	1.00	0.00	A
ATOM	115	C	SER	158	19.764	89.191	14.750	1.00	19.11	A
ATOM	116	O	SER	158	20.168	90.196	15.331	1.00	15.49	A
ATOM	117	N	ILE	159	19.985	88.994	13.462	1.00	19.24	A
ATOM	118	H	ILE	159	19.683	88.164	13.037	1.00	0.00	A
ATOM	119	CA	ILE	159	20.674	90.002	12.670	1.00	24.70	A
ATOM	120	CB	ILE	159	20.702	89.596	11.193	1.00	25.84	A
ATOM	121	CG2	ILE	159	21.185	90.750	10.347	1.00	23.12	A
ATOM	122	CG1	ILE	159	21.602	88.366	11.029	1.00	30.68	A
ATOM	123	CD1	ILE	159	21.058	87.313	10.092	1.00	36.48	A
ATOM	124	C	ILE	159	19.755	91.188	12.863	1.00	29.72	A
ATOM	125	O	ILE	159	18.733	91.293	12.201	1.00	27.59	A
ATOM	126	N	TYR	160	20.099	92.098	13.764	1.00	32.64	A
ATOM	127	H	TYR	160	20.953	92.057	14.240	1.00	0.00	A
ATOM	128	CA	TYR	160	19.142	93.153	13.995	1.00	36.31	A
ATOM	129	CB	TYR	160	19.262	93.759	15.384	1.00	29.60	A
ATOM	130	CG	TYR	160	18.250	94.871	15.541	1.00	25.36	A
ATOM	131	CD1	TYR	160	16.953	94.731	15.034	1.00	30.44	A
ATOM	132	CE1	TYR	160	16.027	95.768	15.113	1.00	28.80	A
ATOM	133	CD2	TYR	160	18.597	96.077	16.131	1.00	22.43	A
ATOM	134	CE2	TYR	160	17.686	97.118	16.218	1.00	29.79	A
ATOM	135	CZ	TYR	160	16.406	96.958	15.706	1.00	29.67	A
ATOM	136	OH	TYR	160	15.514	97.989	15.801	1.00	35.06	A
ATOM	137	HH	TYR	160	14.682	97.730	15.399	1.00	0.00	A
ATOM	138	C	TYR	160	19.015	94.279	13.018	1.00	38.57	A
ATOM	139	O	TYR	160	18.019	94.342	12.297	1.00	45.05	A
ATOM	140	N	PRO	161	19.992	95.194	12.969	1.00	34.46	A
ATOM	141	CD	PRO	161	21.298	95.354	13.624	1.00	23.12	A
ATOM	142	CA	PRO	161	19.727	96.237	11.978	1.00	32.11	A
ATOM	143	CB	PRO	161	20.946	97.155	12.068	1.00	30.05	A
ATOM	144	CG	PRO	161	21.657	96.769	13.287	1.00	34.00	A
ATOM	145	C	PRO	161	19.578	95.579	10.605	1.00	30.24	A
ATOM	146	O	PRO	161	20.555	95.434	9.878	1.00	29.38	A
ATOM	147	N	TRP	162	18.365	95.167	10.254	1.00	28.87	A
ATOM	148	H	TRP	162	17.603	95.296	10.855	1.00	0.00	A
ATOM	149	CA	TRP	162	18.180	94.525	8.970	1.00	29.54	A
ATOM	150	CB	TRP	162	16.725	94.114	8.744	1.00	28.05	A
ATOM	151	CG	TRP	162	16.577	93.324	7.456	1.00	27.54	A
ATOM	152	CD2	TRP	162	17.115	92.017	7.176	1.00	22.18	A
ATOM	153	CE2	TRP	162	16.795	91.710	5.837	1.00	27.60	A
ATOM	154	CE3	TRP	162	17.831	91.081	7.935	1.00	22.75	A

ATOM	155	CD1	TRP	162	15.976	93.740	6.304	1.00	27.18	A
ATOM	156	NE1	TRP	162	16.103	92.779	5.324	1.00	31.45	A
ATOM	157	HE1	TRP	162	15.756	92.847	4.416	1.00	0.00	A
ATOM	158	CZ2	TRP	162	17.169	90.503	5.230	1.00	25.17	A
ATOM	159	CZ3	TRP	162	18.201	89.879	7.343	1.00	21.51	A
ATOM	160	CH2	TRP	162	17.872	89.601	5.998	1.00	27.23	A
ATOM	161	C	TRP	162	18.644	95.419	7.825	1.00	32.23	A
ATOM	162	O	TRP	162	19.318	94.945	6.914	1.00	29.79	A
ATOM	163	N	GLU	163	18.314	96.708	7.859	1.00	34.04	A
ATOM	164	H	GLU	163	17.794	97.072	8.607	1.00	0.00	A
ATOM	165	CA	GLU	163	18.744	97.572	6.757	1.00	36.74	A
ATOM	166	CB	GLU	163	18.235	99.011	6.936	1.00	33.42	A
ATOM	167	CG	GLU	163	17.941	99.437	8.355	1.00	41.87	A
ATOM	168	CD	GLU	163	18.085	100.938	8.529	1.00	43.51	A
ATOM	169	OE1	GLU	163	19.238	101.426	8.588	1.00	44.11	A
ATOM	170	OE2	GLU	163	17.047	101.629	8.597	1.00	39.73	A
ATOM	171	C	GLU	163	20.267	97.578	6.566	1.00	35.78	A
ATOM	172	O	GLU	163	20.769	98.002	5.519	1.00	29.20	A
ATOM	173	N	SER	164	20.987	97.083	7.574	1.00	35.57	A
ATOM	174	H	SER	164	20.516	96.748	8.364	1.00	0.00	A
ATOM	175	CA	SER	164	22.443	97.024	7.547	1.00	31.38	A
ATOM	176	CB	SER	164	22.990	96.956	8.968	1.00	30.80	A
ATOM	177	OG	SER	164	22.876	98.211	9.605	1.00	37.22	A
ATOM	178	HG	SER	164	23.225	98.151	10.498	1.00	0.00	A
ATOM	179	C	SER	164	22.964	95.837	6.751	1.00	32.24	A
ATOM	180	O	SER	164	24.084	95.870	6.231	1.00	37.08	A
ATOM	181	N	VAL	165	22.171	94.775	6.688	1.00	31.62	A
ATOM	182	H	VAL	165	21.316	94.783	7.165	1.00	0.00	A
ATOM	183	CA	VAL	165	22.553	93.602	5.916	1.00	31.01	A
ATOM	184	CB	VAL	165	21.623	92.401	6.164	1.00	35.77	A
ATOM	185	CG1	VAL	165	22.339	91.110	5.787	1.00	39.39	A
ATOM	186	CG2	VAL	165	21.177	92.366	7.607	1.00	40.80	A
ATOM	187	C	VAL	165	22.328	94.049	4.493	1.00	32.48	A
ATOM	188	O	VAL	165	23.156	93.824	3.609	1.00	35.34	A
ATOM	189	N	ILE	166	21.187	94.701	4.297	1.00	33.35	A
ATOM	190	H	ILE	166	20.586	94.837	5.058	1.00	0.00	A
ATOM	191	CA	ILE	166	20.789	95.225	2.997	1.00	32.78	A
ATOM	192	CB	ILE	166	19.382	95.862	3.078	1.00	31.47	A
ATOM	193	CG2	ILE	166	19.056	96.575	1.783	1.00	32.21	A
ATOM	194	CG1	ILE	166	18.346	94.785	3.419	1.00	30.98	A
ATOM	195	CD1	ILE	166	16.917	95.142	3.048	1.00	25.05	A
ATOM	196	C	ILE	166	21.800	96.267	2.504	1.00	30.96	A
ATOM	197	O	ILE	166	22.159	96.293	1.326	1.00	31.98	A
ATOM	198	N	ALA	167	22.260	97.120	3.410	1.00	31.52	A
ATOM	199	H	ALA	167	21.947	97.057	4.337	1.00	0.00	A
ATOM	200	CA	ALA	167	23.228	98.153	3.047	1.00	33.64	A
ATOM	201	CB	ALA	167	23.540	99.023	4.253	1.00	29.88	A
ATOM	202	C	ALA	167	24.502	97.482	2.539	1.00	35.05	A
ATOM	203	O	ALA	167	25.176	97.982	1.630	1.00	30.30	A
ATOM	204	N	PHE	168	24.821	96.342	3.141	1.00	31.11	A
ATOM	205	H	PHE	168	24.245	96.013	3.864	1.00	0.00	A
ATOM	206	CA	PHE	168	25.987	95.572	2.771	1.00	28.96	A
ATOM	207	CB	PHE	168	26.214	94.504	3.835	1.00	32.92	A
ATOM	208	CG	PHE	168	27.007	93.329	3.371	1.00	29.30	A
ATOM	209	CD1	PHE	168	26.378	92.118	3.111	1.00	31.94	A
ATOM	210	CD2	PHE	168	28.386	93.405	3.266	1.00	26.68	A
ATOM	211	CE1	PHE	168	27.104	90.990	2.760	1.00	28.37	A
ATOM	212	CE2	PHE	168	29.128	92.282	2.913	1.00	31.48	A
ATOM	213	CZ	PHE	168	28.481	91.071	2.660	1.00	33.94	A
ATOM	214	C	PHE	168	25.736	94.955	1.395	1.00	30.36	A
ATOM	215	O	PHE	168	26.549	95.106	0.482	1.00	25.57	A
ATOM	216	N	LEU	169	24.602	94.279	1.241	1.00	29.42	A
ATOM	217	H	LEU	169	23.985	94.192	1.997	1.00	0.00	A
ATOM	218	CA	LEU	169	24.262	93.666	-0.037	1.00	32.92	A
ATOM	219	CB	LEU	169	22.835	93.109	-0.008	1.00	30.46	A
ATOM	220	CG	LEU	169	22.485	91.838	0.773	1.00	27.73	A
ATOM	221	CD1	LEU	169	21.107	91.386	0.309	1.00	23.84	A
ATOM	222	CD2	LEU	169	23.504	90.738	0.549	1.00	22.89	A
ATOM	223	C	LEU	169	24.371	94.717	-1.148	1.00	36.13	A
ATOM	224	O	LEU	169	24.992	94.484	-2.181	1.00	37.86	A
ATOM	225	N	ASN	170	23.760	95.876	-0.920	1.00	39.95	A
ATOM	226	H	ASN	170	23.279	95.996	-0.078	1.00	0.00	A
ATOM	227	CA	ASN	170	23.779	96.977	-1.882	1.00	35.60	A

ATOM	228	CB	ASN	170	23.040	98.179	-1.275	1.00	40.87	A
ATOM	229	CG	ASN	170	23.122	99.427	-2.140	1.00	45.43	A
ATOM	230	OD1	ASN	170	24.008	100.268	-1.958	1.00	38.53	A
ATOM	231	ND2	ASN	170	22.191	99.558	-3.083	1.00	44.25	A
ATOM	232	HD21	ASN	170	21.503	98.868	-3.188	1.00	0.00	A
ATOM	233	HD22	ASN	170	22.229	100.355	-3.648	1.00	0.00	A
ATOM	234	C	ASN	170	25.221	97.354	-2.203	1.00	37.08	A
ATOM	235	O	ASN	170	25.590	97.546	-3.360	1.00	36.45	A
ATOM	236	N	ASP	171	26.022	97.444	-1.149	1.00	41.63	A
ATOM	237	H	ASP	171	25.640	97.256	-0.267	1.00	0.00	A
ATOM	238	CA	ASP	171	27.430	97.805	-1.219	1.00	45.96	A
ATOM	239	CB	ASP	171	27.984	97.921	0.205	1.00	49.80	A
ATOM	240	CG	ASP	171	28.976	99.051	0.360	1.00	58.06	A
ATOM	241	OD1	ASP	171	28.606	100.218	0.111	1.00	61.54	A
ATOM	242	OD2	ASP	171	30.131	98.771	0.738	1.00	60.67	A
ATOM	243	C	ASP	171	28.286	96.815	-2.018	1.00	47.51	A
ATOM	244	O	ASP	171	29.263	97.214	-2.656	1.00	45.54	A
ATOM	245	N	LEU	172	27.923	95.535	-1.972	1.00	44.73	A
ATOM	246	H	LEU	172	27.131	95.289	-1.448	1.00	0.00	A
ATOM	247	CA	LEU	172	28.658	94.480	-2.675	1.00	43.36	A
ATOM	248	CB	LEU	172	28.434	93.125	-1.985	1.00	37.47	A
ATOM	249	CG	LEU	172	29.574	92.102	-1.869	1.00	35.42	A
ATOM	250	CD1	LEU	172	29.011	90.764	-1.398	1.00	32.59	A
ATOM	251	CD2	LEU	172	30.274	91.926	-3.189	1.00	32.89	A
ATOM	252	C	LEU	172	28.214	94.362	-4.122	1.00	43.76	A
ATOM	253	O	LEU	172	29.013	94.070	-5.011	1.00	42.82	A
ATOM	254	N	LEU	173	26.928	94.587	-4.345	1.00	45.41	A
ATOM	255	H	LEU	173	26.349	94.834	-3.595	1.00	0.00	A
ATOM	256	CA	LEU	173	26.354	94.481	-5.674	1.00	49.41	A
ATOM	257	CB	LEU	173	24.837	94.308	-5.561	1.00	52.76	A
ATOM	258	CG	LEU	173	24.329	92.938	-5.089	1.00	54.19	A
ATOM	259	CD1	LEU	173	24.148	92.038	-6.294	1.00	59.26	A
ATOM	260	CD2	LEU	173	25.302	92.305	-4.110	1.00	54.13	A
ATOM	261	C	LEU	173	26.681	95.681	-6.552	1.00	51.49	A
ATOM	262	O	LEU	173	27.079	95.521	-7.708	1.00	46.63	A
ATOM	263	N	LYS	174	26.523	96.882	-5.997	1.00	51.16	A
ATOM	264	H	LYS	174	26.220	96.946	-5.068	1.00	0.00	A
ATOM	265	CA	LYS	174	26.794	98.096	-6.751	1.00	51.25	A
ATOM	266	CB	LYS	174	26.615	99.330	-5.862	1.00	50.79	A
ATOM	267	CG	LYS	174	27.294	99.251	-4.513	1.00	49.59	A
ATOM	268	CD	LYS	174	26.659	100.247	-3.542	1.00	48.26	A
ATOM	269	CE	LYS	174	27.707	100.970	-2.714	1.00	41.18	A
ATOM	270	NZ	LYS	174	28.712	101.644	-3.574	1.00	37.27	A
ATOM	271	HZ1	LYS	174	28.236	102.341	-4.183	1.00	0.00	A
ATOM	272	HZ2	LYS	174	29.192	100.937	-4.168	1.00	0.00	A
ATOM	273	HZ3	LYS	174	29.413	102.127	-2.977	1.00	0.00	A
ATOM	274	C	LYS	174	28.181	98.114	-7.384	1.00	48.99	A
ATOM	275	O	LYS	174	28.439	98.906	-8.276	1.00	49.73	A
ATOM	276	N	ARG	175	29.066	97.237	-6.928	1.00	51.76	A
ATOM	277	H	ARG	175	28.807	96.620	-6.212	1.00	0.00	A
ATOM	278	CA	ARG	175	30.422	97.174	-7.471	1.00	54.88	A
ATOM	279	CB	ARG	175	31.400	96.730	-6.378	1.00	60.59	A
ATOM	280	CG	ARG	175	32.257	97.853	-5.813	1.00	69.97	A
ATOM	281	CD	ARG	175	32.030	98.026	-4.320	1.00	76.88	A
ATOM	282	NE	ARG	175	32.502	99.320	-3.832	1.00	82.84	A
ATOM	283	HE	ARG	175	33.238	99.324	-3.186	1.00	0.00	A
ATOM	284	CZ	ARG	175	31.996	100.490	-4.208	1.00	86.91	A
ATOM	285	NH1	ARG	175	30.996	100.535	-5.080	1.00	88.00	A
ATOM	286	HH11	ARG	175	30.620	99.687	-5.452	1.00	0.00	A
ATOM	287	HH12	ARG	175	30.617	101.416	-5.361	1.00	0.00	A
ATOM	288	NH2	ARG	175	32.492	101.619	-3.712	1.00	88.60	A
ATOM	289	HH21	ARG	175	33.245	101.588	-3.054	1.00	0.00	A
ATOM	290	HH22	ARG	175	32.112	102.499	-3.996	1.00	0.00	A
ATOM	291	C	ARG	175	30.543	96.231	-8.675	1.00	52.71	A
ATOM	292	O	ARG	175	31.308	96.486	-9.604	1.00	51.98	A
ATOM	293	N	MET	176	29.777	95.147	-8.654	1.00	49.83	A
ATOM	294	H	MET	176	29.175	95.007	-7.894	1.00	0.00	A
ATOM	295	CA	MET	176	29.805	94.159	-9.720	1.00	44.82	A
ATOM	296	CB	MET	176	29.033	92.907	-9.306	1.00	39.16	A
ATOM	297	CG	MET	176	29.372	92.339	-7.956	1.00	37.27	A
ATOM	298	SD	MET	176	28.290	90.955	-7.596	1.00	40.47	A
ATOM	299	CE	MET	176	29.105	90.252	-6.182	1.00	36.51	A
ATOM	300	C	MET	176	29.208	94.651	-11.028	1.00	47.84	A

```
ATOM    301  O   MET   176      28.361  95.542 -11.049  1.00 46.58      A
ATOM    302  N   ASP   177      29.656  94.035 -12.118  1.00 51.49      A
ATOM    303  H   ASP   177      30.352  93.353 -12.016  1.00  0.00      A
ATOM    304  CA  ASP   177      29.157  94.329 -13.457  1.00 54.36      A
ATOM    305  CB  ASP   177      30.322  94.519 -14.441  1.00 56.10      A
ATOM    306  CG  ASP   177      30.746  95.974 -14.586  1.00 60.14      A
ATOM    307  OD1 ASP   177      31.960  96.219 -14.732  1.00 58.72      A
ATOM    308  OD2 ASP   177      29.874  96.868 -14.559  1.00 61.23      A
ATOM    309  C   ASP   177      28.366  93.070 -13.833  1.00 54.37      A
ATOM    310  O   ASP   177      28.944  92.089 -14.304  1.00 54.71      A
ATOM    311  N   ILE   178      27.056  93.088 -13.603  1.00 50.87      A
ATOM    312  H   ILE   178      26.644  93.892 -13.226  1.00  0.00      A
ATOM    313  CA  ILE   178      26.220  91.929 -13.905  1.00 50.24      A
ATOM    314  CB  ILE   178      24.921  91.933 -13.041  1.00 49.66      A
ATOM    315  CG2 ILE   178      24.214  90.581 -13.131  1.00 49.10      A
ATOM    316  CG1 ILE   178      25.275  92.217 -11.576  1.00 50.99      A
ATOM    317  CD1 ILE   178      24.125  92.001 -10.593  1.00 52.23      A
ATOM    318  C   ILE   178      25.855  91.871 -15.386  1.00 48.57      A
ATOM    319  O   ILE   178      25.743  92.905 -16.040  1.00 50.81      A
ATOM    320  N   GLY   179      25.689  90.654 -15.902  1.00 48.26      A
ATOM    321  H   GLY   179      25.801  89.873 -15.324  1.00  0.00      A
ATOM    322  CA  GLY   179      25.341  90.453 -17.300  1.00 47.18      A
ATOM    323  C   GLY   179      25.483  88.993 -17.708  1.00 47.42      A
ATOM    324  O   GLY   179      26.366  88.302 -17.203  1.00 44.46      A
ATOM    325  N   PRO   180      24.635  88.489 -18.621  1.00 48.62      A
ATOM    326  CD  PRO   180      23.543  89.194 -19.313  1.00 50.81      A
ATOM    327  CA  PRO   180      24.730  87.084 -19.046  1.00 49.53      A
ATOM    328  CB  PRO   180      23.635  86.946 -20.107  1.00 48.70      A
ATOM    329  CG  PRO   180      22.692  88.070 -19.837  1.00 52.71      A
ATOM    330  C   PRO   180      26.104  86.712 -19.597  1.00 52.68      A
ATOM    331  O   PRO   180      26.359  85.541 -19.902  1.00 53.20      A
ATOM    332  N   LYS   181      26.983  87.706 -19.716  1.00 49.61      A
ATOM    333  H   LYS   181      26.720  88.610 -19.445  1.00  0.00      A
ATOM    334  CA  LYS   181      28.324  87.485 -20.238  1.00 49.94      A
ATOM    335  CB  LYS   181      28.517  88.279 -21.535  1.00 52.40      A
ATOM    336  CG  LYS   181      27.413  88.064 -22.577  1.00 52.89      A
ATOM    337  CD  LYS   181      27.111  86.588 -22.801  1.00 50.48      A
ATOM    338  CE  LYS   181      28.125  85.942 -23.735  1.00 54.32      A
ATOM    339  NZ  LYS   181      29.156  85.176 -22.981  1.00 54.02      A
ATOM    340  HZ1 LYS   181      28.696  84.425 -22.427  1.00  0.00      A
ATOM    341  HZ2 LYS   181      29.664  85.818 -22.338  1.00  0.00      A
ATOM    342  HZ3 LYS   181      29.830  84.750 -23.648  1.00  0.00      A
ATOM    343  C   LYS   181      29.389  87.882 -19.223  1.00 49.03      A
ATOM    344  O   LYS   181      30.575  87.943 -19.544  1.00 44.77      A
ATOM    345  N   GLN   182      28.953  88.150 -17.997  1.00 49.13      A
ATOM    346  H   GLN   182      27.997  88.071 -17.806  1.00  0.00      A
ATOM    347  CA  GLN   182      29.855  88.549 -16.927  1.00 47.58      A
ATOM    348  CB  GLN   182      30.657  89.802 -17.332  1.00 52.30      A
ATOM    349  CG  GLN   182      29.961  91.148 -17.105  1.00 56.19      A
ATOM    350  CD  GLN   182      29.400  91.760 -18.381  1.00 59.68      A
ATOM    351  OE1 GLN   182      28.651  92.742 -18.337  1.00 59.75      A
ATOM    352  NE2 GLN   182      29.759  91.184 -19.526  1.00 62.02      A
ATOM    353 HE21 GLN   182      30.356  90.408 -19.515  1.00  0.00      A
ATOM    354 HE22 GLN   182      29.407  91.567 -20.355  1.00  0.00      A
ATOM    355  C   GLN   182      29.039  88.817 -15.673  1.00 46.05      A
ATOM    356  O   GLN   182      28.205  89.720 -15.635  1.00 52.56      A
ATOM    357  N   THR   183      29.279  88.007 -14.655  1.00 43.42      A
ATOM    358  H   THR   183      29.952  87.304 -14.768  1.00  0.00      A
ATOM    359  CA  THR   183      28.590  88.107 -13.367  1.00 39.86      A
ATOM    360  CB  THR   183      28.994  89.369 -12.571  1.00 38.78      A
ATOM    361  OG1 THR   183      30.422  89.443 -12.473  1.00 33.64      A
ATOM    362  HG1 THR   183      30.753  88.664 -12.022  1.00  0.00      A
ATOM    363  CG2 THR   183      28.407  89.303 -11.165  1.00 36.70      A
ATOM    364  C   THR   183      27.073  88.054 -13.388  1.00 40.16      A
ATOM    365  O   THR   183      26.397  88.889 -14.001  1.00 37.82      A
ATOM    366  N   GLN   184      26.565  87.044 -12.692  1.00 38.77      A
ATOM    367  H   GLN   184      27.185  86.424 -12.260  1.00  0.00      A
ATOM    368  CA  GLN   184      25.148  86.805 -12.534  1.00 32.70      A
ATOM    369  CB  GLN   184      24.755  85.500 -13.199  1.00 39.22      A
ATOM    370  CG  GLN   184      24.950  85.502 -14.684  1.00 38.77      A
ATOM    371  CD  GLN   184      23.866  84.736 -15.379  1.00 37.99      A
ATOM    372  OE1 GLN   184      23.633  83.563 -15.081  1.00 34.86      A
ATOM    373  NE2 GLN   184      23.182  85.395 -16.306  1.00 36.73      A
```

ATOM	374	HE21	GLN	184	23.400	86.330	-16.503	1.00	0.00	A
ATOM	375	HE22	GLN	184	22.470	84.910	-16.770	1.00	0.00	A
ATOM	376	C	GLN	184	24.956	86.687	-11.032	1.00	34.89	A
ATOM	377	O	GLN	184	25.816	86.138	-10.331	1.00	31.60	A
ATOM	378	N	VAL	185	23.819	87.185	-10.552	1.00	35.52	A
ATOM	379	H	VAL	185	23.168	87.567	-11.175	1.00	0.00	A
ATOM	380	CA	VAL	185	23.510	87.179	-9.129	1.00	33.81	A
ATOM	381	CB	VAL	185	23.602	88.617	-8.545	1.00	35.05	A
ATOM	382	CG1	VAL	185	23.088	88.636	-7.094	1.00	35.71	A
ATOM	383	CG2	VAL	185	25.048	89.115	-8.612	1.00	16.86	A
ATOM	384	C	VAL	185	22.137	86.604	-8.772	1.00	34.96	A
ATOM	385	O	VAL	185	21.129	86.859	-9.441	1.00	29.48	A
ATOM	386	N	GLY	186	22.129	85.830	-7.691	1.00	29.37	A
ATOM	387	H	GLY	186	22.968	85.675	-7.209	1.00	0.00	A
ATOM	388	CA	GLY	186	20.915	85.215	-7.208	1.00	33.55	A
ATOM	389	C	GLY	186	20.922	85.345	-5.706	1.00	30.62	A
ATOM	390	O	GLY	186	21.978	85.507	-5.092	1.00	38.55	A
ATOM	391	N	ILE	187	19.751	85.285	-5.100	1.00	29.16	A
ATOM	392	H	ILE	187	18.935	85.152	-5.626	1.00	0.00	A
ATOM	393	CA	ILE	187	19.667	85.411	-3.657	1.00	29.27	A
ATOM	394	CB	ILE	187	19.244	86.832	-3.222	1.00	23.80	A
ATOM	395	CG2	ILE	187	19.187	86.902	-1.708	1.00	21.78	A
ATOM	396	CG1	ILE	187	20.223	87.869	-3.771	1.00	25.79	A
ATOM	397	CD1	ILE	187	20.020	89.264	-3.200	1.00	26.87	A
ATOM	398	C	ILE	187	18.656	84.456	-3.063	1.00	28.09	A
ATOM	399	O	ILE	187	17.537	84.337	-3.549	1.00	26.92	A
ATOM	400	N	VAL	188	19.057	83.793	-1.989	1.00	31.92	A
ATOM	401	H	VAL	188	19.971	83.924	-1.660	1.00	0.00	A
ATOM	402	CA	VAL	188	18.175	82.877	-1.288	1.00	31.88	A
ATOM	403	CB	VAL	188	18.598	81.408	-1.538	1.00	30.39	A
ATOM	404	CG1	VAL	188	18.918	80.702	-0.221	1.00	23.72	A
ATOM	405	CG2	VAL	188	17.478	80.688	-2.276	1.00	31.57	A
ATOM	406	C	VAL	188	18.271	83.226	0.198	1.00	30.17	A
ATOM	407	O	VAL	188	19.362	83.436	0.719	1.00	29.85	A
ATOM	408	N	GLN	189	17.132	83.332	0.869	1.00	26.31	A
ATOM	409	H	GLN	189	16.278	83.201	0.405	1.00	0.00	A
ATOM	410	CA	GLN	189	17.146	83.644	2.288	1.00	27.42	A
ATOM	411	CB	GLN	189	16.219	84.830	2.629	1.00	25.02	A
ATOM	412	CG	GLN	189	16.196	85.140	4.141	1.00	21.62	A
ATOM	413	CD	GLN	189	15.631	86.506	4.495	1.00	22.57	A
ATOM	414	OE1	GLN	189	15.554	86.867	5.668	1.00	23.48	A
ATOM	415	NE2	GLN	189	15.230	87.263	3.487	1.00	26.01	A
ATOM	416	HE21	GLN	189	15.304	86.940	2.567	1.00	0.00	A
ATOM	417	HE22	GLN	189	14.866	88.147	3.709	1.00	0.00	A
ATOM	418	C	GLN	189	16.679	82.392	3.000	1.00	23.00	A
ATOM	419	O	GLN	189	15.882	81.631	2.463	1.00	23.43	A
ATOM	420	N	TYR	190	17.184	82.171	4.202	1.00	22.53	A
ATOM	421	H	TYR	190	17.820	82.811	4.584	1.00	0.00	A
ATOM	422	CA	TYR	190	16.811	80.993	4.963	1.00	26.52	A
ATOM	423	CB	TYR	190	17.837	79.883	4.726	1.00	26.90	A
ATOM	424	CG	TYR	190	19.147	80.113	5.453	1.00	17.55	A
ATOM	425	CD1	TYR	190	19.397	79.503	6.676	1.00	15.45	A
ATOM	426	CE1	TYR	190	20.593	79.699	7.345	1.00	17.09	A
ATOM	427	CD2	TYR	190	20.139	80.936	4.907	1.00	14.28	A
ATOM	428	CE2	TYR	190	21.347	81.138	5.568	1.00	14.48	A
ATOM	429	CZ	TYR	190	21.567	80.513	6.786	1.00	15.88	A
ATOM	430	OH	TYR	190	22.749	80.701	7.467	1.00	15.41	A
ATOM	431	HH	TYR	190	23.313	81.297	6.966	1.00	0.00	A
ATOM	432	C	TYR	190	16.694	81.265	6.463	1.00	28.88	A
ATOM	433	O	TYR	190	17.147	82.297	6.974	1.00	27.66	A
ATOM	434	N	GLY	191	16.093	80.302	7.152	1.00	29.28	A
ATOM	435	H	GLY	191	15.773	79.511	6.669	1.00	0.00	A
ATOM	436	CA	GLY	191	15.888	80.359	8.587	1.00	26.48	A
ATOM	437	C	GLY	191	14.655	79.507	8.787	1.00	27.88	A
ATOM	438	O	GLY	191	13.548	79.953	8.494	1.00	33.37	A
ATOM	439	N	GLU	192	14.843	78.283	9.266	1.00	31.94	A
ATOM	440	H	GLU	192	15.753	78.004	9.499	1.00	0.00	A
ATOM	441	CA	GLU	192	13.744	77.334	9.461	1.00	34.41	A
ATOM	442	CB	GLU	192	12.504	78.026	10.025	1.00	39.00	A
ATOM	443	CG	GLU	192	12.439	78.147	11.534	1.00	39.53	A
ATOM	444	CD	GLU	192	11.319	79.079	11.967	1.00	39.25	A
ATOM	445	OE1	GLU	192	11.611	80.085	12.645	1.00	42.52	A
ATOM	446	OE2	GLU	192	10.146	78.813	11.616	1.00	34.89	A

ATOM	447	C	GLU	192	13.384	76.697	8.111	1.00	34.47	A
ATOM	448	O	GLU	192	13.208	75.487	8.010	1.00	36.09	A
ATOM	449	N	ASN	193	13.265	77.528	7.082	1.00	33.33	A
ATOM	450	H	ASN	193	13.403	78.487	7.234	1.00	0.00	A
ATOM	451	CA	ASN	193	12.935	77.071	5.736	1.00	35.22	A
ATOM	452	CB	ASN	193	11.409	77.105	5.534	1.00	38.44	A
ATOM	453	CG	ASN	193	10.967	78.108	4.484	1.00	42.52	A
ATOM	454	OD1	ASN	193	10.607	77.735	3.366	1.00	48.03	A
ATOM	455	ND2	ASN	193	10.987	79.383	4.840	1.00	45.99	A
ATOM	456	HD21	ASN	193	11.275	79.633	5.739	1.00	0.00	A
ATOM	457	HD22	ASN	193	10.705	80.040	4.172	1.00	0.00	A
ATOM	458	C	ASN	193	13.674	77.964	4.718	1.00	31.48	A
ATOM	459	O	ASN	193	14.389	78.885	5.114	1.00	32.85	A
ATOM	460	N	VAL	194	13.516	77.699	3.423	1.00	28.41	A
ATOM	461	H	VAL	194	12.921	76.971	3.148	1.00	0.00	A
ATOM	462	CA	VAL	194	14.216	78.485	2.408	1.00	30.39	A
ATOM	463	CB	VAL	194	15.300	77.621	1.682	1.00	35.86	A
ATOM	464	CG1	VAL	194	16.253	78.517	0.890	1.00	34.87	A
ATOM	465	CG2	VAL	194	16.086	76.798	2.700	1.00	31.70	A
ATOM	466	C	VAL	194	13.312	79.100	1.347	1.00	26.35	A
ATOM	467	O	VAL	194	12.352	78.487	0.911	1.00	25.27	A
ATOM	468	N	THR	195	13.629	80.327	0.938	1.00	30.82	A
ATOM	469	H	THR	195	14.396	80.780	1.344	1.00	0.00	A
ATOM	470	CA	THR	195	12.861	81.013	-0.097	1.00	32.80	A
ATOM	471	CB	THR	195	11.875	82.059	0.520	1.00	32.61	A
ATOM	472	OG1	THR	195	12.435	83.370	0.439	1.00	36.07	A
ATOM	473	HG1	THR	195	11.821	84.005	0.819	1.00	0.00	A
ATOM	474	CG2	THR	195	11.581	81.730	1.969	1.00	35.80	A
ATOM	475	C	THR	195	13.832	81.698	-1.066	1.00	34.36	A
ATOM	476	O	THR	195	14.830	82.274	-0.638	1.00	37.20	A
ATOM	477	N	HIS	196	13.562	81.610	-2.368	1.00	31.83	A
ATOM	478	H	HIS	196	12.767	81.117	-2.664	1.00	0.00	A
ATOM	479	CA	HIS	196	14.430	82.235	-3.364	1.00	33.42	A
ATOM	480	CB	HIS	196	14.373	81.488	-4.703	1.00	36.34	A
ATOM	481	CG	HIS	196	14.682	80.027	-4.612	1.00	32.56	A
ATOM	482	CD2	HIS	196	13.920	78.975	-4.231	1.00	33.30	A
ATOM	483	ND1	HIS	196	15.885	79.493	-5.025	1.00	30.72	A
ATOM	484	HD1	HIS	196	16.646	80.005	-5.357	1.00	0.00	A
ATOM	485	CE1	HIS	196	15.850	78.181	-4.905	1.00	27.16	A
ATOM	486	NE2	HIS	196	14.669	77.839	-4.425	1.00	24.32	A
ATOM	487	HE2	HIS	196	14.366	76.932	-4.234	1.00	0.00	A
ATOM	488	C	HIS	196	13.990	83.676	-3.600	1.00	33.69	A
ATOM	489	O	HIS	196	12.907	83.910	-4.147	1.00	30.28	A
ATOM	490	N	GLU	197	14.825	84.633	-3.193	1.00	32.40	A
ATOM	491	H	GLU	197	15.670	84.376	-2.769	1.00	0.00	A
ATOM	492	CA	GLU	197	14.522	86.053	-3.357	1.00	28.21	A
ATOM	493	CB	GLU	197	15.485	86.884	-2.515	1.00	30.79	A
ATOM	494	CG	GLU	197	15.369	86.601	-1.025	1.00	29.25	A
ATOM	495	CD	GLU	197	13.980	86.880	-0.489	1.00	28.81	A
ATOM	496	OE1	GLU	197	13.154	87.429	-1.246	1.00	27.20	A
ATOM	497	OE2	GLU	197	13.712	86.550	0.688	1.00	31.09	A
ATOM	498	C	GLU	197	14.578	86.469	-4.831	1.00	25.47	A
ATOM	499	O	GLU	197	13.872	87.380	-5.250	1.00	33.41	A
ATOM	500	N	PHE	198	15.447	85.817	-5.594	1.00	28.05	A
ATOM	501	H	PHE	198	16.035	85.161	-5.166	1.00	0.00	A
ATOM	502	CA	PHE	198	15.573	86.023	-7.038	1.00	29.94	A
ATOM	503	CB	PHE	198	15.668	87.522	-7.420	1.00	22.28	A
ATOM	504	CG	PHE	198	16.939	88.213	-7.021	1.00	20.44	A
ATOM	505	CD1	PHE	198	18.134	87.969	-7.696	1.00	29.59	A
ATOM	506	CD2	PHE	198	16.925	89.166	-6.015	1.00	12.83	A
ATOM	507	CE1	PHE	198	19.300	88.669	-7.376	1.00	23.18	A
ATOM	508	CE2	PHE	198	18.074	89.872	-5.683	1.00	23.57	A
ATOM	509	CZ	PHE	198	19.269	89.626	-6.364	1.00	26.69	A
ATOM	510	C	PHE	198	16.684	85.181	-7.679	1.00	34.58	A
ATOM	511	O	PHE	198	17.787	85.048	-7.131	1.00	35.32	A
ATOM	512	N	ASN	199	16.352	84.590	-8.828	1.00	33.63	A
ATOM	513	H	ASN	199	15.456	84.756	-9.187	1.00	0.00	A
ATOM	514	CA	ASN	199	17.237	83.708	-9.592	1.00	33.60	A
ATOM	515	CB	ASN	199	16.416	82.890	-10.596	1.00	33.43	A
ATOM	516	CG	ASN	199	15.406	81.979	-9.929	1.00	35.08	A
ATOM	517	OD1	ASN	199	15.458	81.743	-8.724	1.00	37.14	A
ATOM	518	ND2	ASN	199	14.480	81.457	-10.717	1.00	36.96	A
ATOM	519	HD21	ASN	199	14.477	81.669	-11.674	1.00	0.00	A

```
ATOM    520 HD22 ASN   199      13.818  80.865 -10.306  1.00  0.00      A
ATOM    521  C   ASN   199      18.381  84.392 -10.352  1.00 37.18      A
ATOM    522  O   ASN   199      18.312  85.573 -10.690  1.00 33.75      A
ATOM    523  N   LEU   200      19.413  83.605 -10.649  1.00 35.28      A
ATOM    524  H   LEU   200      19.374  82.663 -10.382  1.00  0.00      A
ATOM    525  CA  LEU   200      20.595  84.080 -11.357  1.00 36.97      A
ATOM    526  CB  LEU   200      21.612  82.943 -11.502  1.00 36.01      A
ATOM    527  CG  LEU   200      22.358  82.306 -10.328  1.00 32.50      A
ATOM    528  CD1 LEU   200      21.430  81.966  -9.168  1.00 38.36      A
ATOM    529  CD2 LEU   200      22.997  81.034 -10.851  1.00 33.04      A
ATOM    530  C   LEU   200      20.304  84.640 -12.746  1.00 36.89      A
ATOM    531  O   LEU   200      21.069  85.453 -13.256  1.00 38.59      A
ATOM    532  N   ASN   201      19.217  84.196 -13.370  1.00 38.74      A
ATOM    533  H   ASN   201      18.633  83.546 -12.929  1.00  0.00      A
ATOM    534  CA  ASN   201      18.891  84.676 -14.713  1.00 40.95      A
ATOM    535  CB  ASN   201      18.643  83.497 -15.666  1.00 42.74      A
ATOM    536  CG  ASN   201      17.424  82.664 -15.284  1.00 45.08      A
ATOM    537  OD1 ASN   201      17.100  81.693 -15.969  1.00 46.68      A
ATOM    538  ND2 ASN   201      16.746  83.032 -14.199  1.00 42.33      A
ATOM    539 HD21 ASN   201      17.038  83.811 -13.682  1.00  0.00      A
ATOM    540 HD22 ASN   201      15.963  82.499 -13.952  1.00  0.00      A
ATOM    541  C   ASN   201      17.696  85.616 -14.726  1.00 41.99      A
ATOM    542  O   ASN   201      17.194  85.997 -15.785  1.00 36.95      A
ATOM    543  N   LYS   202      17.257  85.993 -13.532  1.00 43.02      A
ATOM    544  H   LYS   202      17.711  85.657 -12.731  1.00  0.00      A
ATOM    545  CA  LYS   202      16.127  86.889 -13.378  1.00 42.25      A
ATOM    546  CB  LYS   202      15.743  86.957 -11.896  1.00 37.84      A
ATOM    547  CG  LYS   202      14.984  88.195 -11.505  1.00 39.09      A
ATOM    548  CD  LYS   202      13.486  88.011 -11.664  1.00 41.90      A
ATOM    549  CE  LYS   202      12.851  87.494 -10.381  1.00 47.46      A
ATOM    550  NZ  LYS   202      12.961  86.005 -10.253  1.00 45.02      A
ATOM    551  HZ1 LYS   202      13.963  85.729 -10.250  1.00  0.00      A
ATOM    552  HZ2 LYS   202      12.479  85.552 -11.057  1.00  0.00      A
ATOM    553  HZ3 LYS   202      12.513  85.699  -9.366  1.00  0.00      A
ATOM    554  C   LYS   202      16.443  88.287 -13.921  1.00 40.53      A
ATOM    555  O   LYS   202      15.698  88.829 -14.735  1.00 36.63      A
ATOM    556  N   TYR   203      17.558  88.864 -13.486  1.00 41.00      A
ATOM    557  H   TYR   203      18.140  88.383 -12.861  1.00  0.00      A
ATOM    558  CA  TYR   203      17.923  90.201 -13.931  1.00 40.78      A
ATOM    559  CB  TYR   203      18.101  91.114 -12.711  1.00 43.99      A
ATOM    560  CG  TYR   203      16.946  91.108 -11.723  1.00 42.62      A
ATOM    561  CD1 TYR   203      17.064  90.475 -10.483  1.00 42.17      A
ATOM    562  CE1 TYR   203      16.027  90.492  -9.556  1.00 36.22      A
ATOM    563  CD2 TYR   203      15.750  91.761 -12.010  1.00 44.83      A
ATOM    564  CE2 TYR   203      14.702  91.786 -11.086  1.00 48.25      A
ATOM    565  CZ  TYR   203      14.848  91.151  -9.860  1.00 47.45      A
ATOM    566  OH  TYR   203      13.815  91.181  -8.942  1.00 52.58      A
ATOM    567  HH  TYR   203      13.077  91.678  -9.304  1.00  0.00      A
ATOM    568  C   TYR   203      19.181  90.243 -14.813  1.00 42.72      A
ATOM    569  O   TYR   203      20.014  89.335 -14.784  1.00 38.83      A
ATOM    570  N   SER   204      19.313  91.312 -15.591  1.00 43.42      A
ATOM    571  H   SER   204      18.628  92.013 -15.556  1.00  0.00      A
ATOM    572  CA  SER   204      20.445  91.476 -16.499  1.00 45.46      A
ATOM    573  CB  SER   204      19.945  91.613 -17.933  1.00 47.15      A
ATOM    574  OG  SER   204      19.893  92.982 -18.309  1.00 49.62      A
ATOM    575  HG  SER   204      20.770  93.366 -18.244  1.00  0.00      A
ATOM    576  C   SER   204      21.312  92.691 -16.188  1.00 49.08      A
ATOM    577  O   SER   204      22.464  92.760 -16.616  1.00 48.50      A
ATOM    578  N   SER   205      20.757  93.656 -15.462  1.00 50.50      A
ATOM    579  H   SER   205      19.839  93.549 -15.138  1.00  0.00      A
ATOM    580  CA  SER   205      21.495  94.870 -15.141  1.00 49.60      A
ATOM    581  CB  SER   205      20.634  96.098 -15.449  1.00 49.35      A
ATOM    582  OG  SER   205      21.303  96.970 -16.345  1.00 54.35      A
ATOM    583  HG  SER   205      22.128  97.262 -15.950  1.00  0.00      A
ATOM    584  C   SER   205      21.981  94.944 -13.699  1.00 47.82      A
ATOM    585  O   SER   205      21.316  94.469 -12.785  1.00 41.96      A
ATOM    586  N   THR   206      23.151  95.547 -13.512  1.00 46.13      A
ATOM    587  H   THR   206      23.643  95.889 -14.287  1.00  0.00      A
ATOM    588  CA  THR   206      23.715  95.710 -12.184  1.00 49.52      A
ATOM    589  CB  THR   206      25.121  96.351 -12.233  1.00 46.33      A
ATOM    590  OG1 THR   206      26.115  95.324 -12.316  1.00 47.49      A
ATOM    591  HG1 THR   206      26.050  94.753 -11.545  1.00  0.00      A
ATOM    592  CG2 THR   206      25.381  97.172 -10.980  1.00 46.12      A
```

ATOM	593	C	THR	206	22.792	96.617	-11.383	1.00	49.12	A
ATOM	594	O	THR	206	22.684	96.479	-10.166	1.00	53.03	A
ATOM	595	N	GLU	207	22.123	97.538	-12.070	1.00	51.42	A
ATOM	596	H	GLU	207	22.243	97.592	-13.042	1.00	0.00	A
ATOM	597	CA	GLU	207	21.215	98.469	-11.408	1.00	49.16	A
ATOM	598	CB	GLU	207	21.002	99.720	-12.269	1.00	52.87	A
ATOM	599	CG	GLU	207	21.187	99.521	-13.762	1.00	55.52	A
ATOM	600	CD	GLU	207	20.886	100.782	-14.550	1.00	56.44	A
ATOM	601	OE1	GLU	207	21.844	101.489	-14.932	1.00	55.48	A
ATOM	602	OE2	GLU	207	19.692	101.066	-14.784	1.00	53.55	A
ATOM	603	C	GLU	207	19.864	97.858	-11.066	1.00	49.23	A
ATOM	604	O	GLU	207	19.350	98.053	-9.964	1.00	48.23	A
ATOM	605	N	GLU	208	19.276	97.122	-12.000	1.00	47.83	A
ATOM	606	H	GLU	208	19.710	96.988	-12.870	1.00	0.00	A
ATOM	607	CA	GLU	208	17.981	96.511	-11.727	1.00	48.69	A
ATOM	608	CB	GLU	208	17.500	95.700	-12.916	1.00	45.35	A
ATOM	609	CG	GLU	208	17.020	96.510	-14.082	1.00	40.10	A
ATOM	610	CD	GLU	208	16.724	95.620	-15.262	1.00	37.99	A
ATOM	611	OE1	GLU	208	15.676	95.799	-15.918	1.00	46.28	A
ATOM	612	OE2	GLU	208	17.545	94.727	-15.528	1.00	36.45	A
ATOM	613	C	GLU	208	18.129	95.584	-10.535	1.00	50.21	A
ATOM	614	O	GLU	208	17.317	95.603	-9.608	1.00	50.81	A
ATOM	615	N	VAL	209	19.174	94.764	-10.573	1.00	47.53	A
ATOM	616	H	VAL	209	19.778	94.788	-11.344	1.00	0.00	A
ATOM	617	CA	VAL	209	19.436	93.832	-9.489	1.00	48.06	A
ATOM	618	CB	VAL	209	20.744	93.024	-9.738	1.00	48.35	A
ATOM	619	CG1	VAL	209	21.363	92.582	-8.421	1.00	49.78	A
ATOM	620	CG2	VAL	209	20.446	91.809	-10.589	1.00	49.88	A
ATOM	621	C	VAL	209	19.549	94.619	-8.187	1.00	45.25	A
ATOM	622	O	VAL	209	19.145	94.138	-7.134	1.00	43.45	A
ATOM	623	N	LEU	210	20.081	95.836	-8.263	1.00	45.57	A
ATOM	624	H	LEU	210	20.373	96.189	-9.130	1.00	0.00	A
ATOM	625	CA	LEU	210	20.232	96.652	-7.061	1.00	46.10	A
ATOM	626	CB	LEU	210	21.031	97.931	-7.356	1.00	44.07	A
ATOM	627	CG	LEU	210	22.557	97.828	-7.549	1.00	44.26	A
ATOM	628	CD1	LEU	210	23.131	99.226	-7.738	1.00	38.37	A
ATOM	629	CD2	LEU	210	23.218	97.138	-6.361	1.00	35.26	A
ATOM	630	C	LEU	210	18.862	97.006	-6.490	1.00	44.20	A
ATOM	631	O	LEU	210	18.653	96.925	-5.286	1.00	44.77	A
ATOM	632	N	VAL	211	17.928	97.389	-7.349	1.00	45.51	A
ATOM	633	H	VAL	211	18.137	97.445	-8.305	1.00	0.00	A
ATOM	634	CA	VAL	211	16.591	97.731	-6.880	1.00	44.84	A
ATOM	635	CB	VAL	211	15.685	98.253	-8.021	1.00	44.98	A
ATOM	636	CG1	VAL	211	14.649	99.213	-7.449	1.00	49.23	A
ATOM	637	CG2	VAL	211	16.517	98.940	-9.095	1.00	47.62	A
ATOM	638	C	VAL	211	15.914	96.503	-6.278	1.00	42.72	A
ATOM	639	O	VAL	211	15.219	96.595	-5.262	1.00	42.50	A
ATOM	640	N	ALA	212	16.122	95.353	-6.907	1.00	40.62	A
ATOM	641	H	ALA	212	16.699	95.334	-7.699	1.00	0.00	A
ATOM	642	CA	ALA	212	15.509	94.116	-6.440	1.00	40.77	A
ATOM	643	CB	ALA	212	15.742	93.011	-7.454	1.00	36.33	A
ATOM	644	C	ALA	212	16.001	93.672	-5.063	1.00	38.58	A
ATOM	645	O	ALA	212	15.207	93.243	-4.221	1.00	37.62	A
ATOM	646	N	ALA	213	17.305	93.779	-4.837	1.00	31.59	A
ATOM	647	H	ALA	213	17.889	94.145	-5.532	1.00	0.00	A
ATOM	648	CA	ALA	213	17.879	93.359	-3.564	1.00	35.24	A
ATOM	649	CB	ALA	213	19.386	93.229	-3.687	1.00	35.74	A
ATOM	650	C	ALA	213	17.540	94.277	-2.404	1.00	33.73	A
ATOM	651	O	ALA	213	17.515	93.837	-1.264	1.00	30.39	A
ATOM	652	N	ASN	214	17.277	95.548	-2.688	1.00	37.82	A
ATOM	653	H	ASN	214	17.292	95.854	-3.618	1.00	0.00	A
ATOM	654	CA	ASN	214	16.962	96.495	-1.620	1.00	41.93	A
ATOM	655	CB	ASN	214	17.152	97.935	-2.102	1.00	43.82	A
ATOM	656	CG	ASN	214	18.495	98.509	-1.688	1.00	45.59	A
ATOM	657	OD1	ASN	214	19.426	98.581	-2.492	1.00	47.44	A
ATOM	658	ND2	ASN	214	18.606	98.911	-0.425	1.00	46.09	A
ATOM	659	HD21	ASN	214	17.842	98.829	0.183	1.00	0.00	A
ATOM	660	HD22	ASN	214	19.465	99.284	-0.143	1.00	0.00	A
ATOM	661	C	ASN	214	15.555	96.313	-1.084	1.00	44.23	A
ATOM	662	O	ASN	214	15.232	96.808	-0.009	1.00	45.11	A
ATOM	663	N	LYS	215	14.724	95.589	-1.830	1.00	44.69	A
ATOM	664	H	LYS	215	15.045	95.212	-2.677	1.00	0.00	A
ATOM	665	CA	LYS	215	13.351	95.347	-1.416	1.00	43.68	A

ATOM	666	CB	LYS	215	12.425	95.401	-2.632	1.00	45.74	A
ATOM	667	CG	LYS	215	12.506	94.172	-3.524	1.00	54.82	A
ATOM	668	CD	LYS	215	12.162	94.511	-4.971	1.00	55.87	A
ATOM	669	CE	LYS	215	11.845	93.258	-5.776	1.00	59.40	A
ATOM	670	NZ	LYS	215	10.388	92.928	-5.762	1.00	58.33	A
ATOM	671	HZ1	LYS	215	9.850	93.718	-6.173	1.00	0.00	A
ATOM	672	HZ2	LYS	215	10.077	92.768	-4.784	1.00	0.00	A
ATOM	673	HZ3	LYS	215	10.223	92.068	-6.323	1.00	0.00	A
ATOM	674	C	LYS	215	13.184	94.007	-0.701	1.00	41.09	A
ATOM	675	O	LYS	215	12.073	93.505	-0.575	1.00	41.46	A
ATOM	676	N	ILE	216	14.280	93.427	-0.227	1.00	38.99	A
ATOM	677	H	ILE	216	15.151	93.863	-0.342	1.00	0.00	A
ATOM	678	CA	ILE	216	14.197	92.146	0.463	1.00	34.14	A
ATOM	679	CB	ILE	216	15.477	91.305	0.281	1.00	34.52	A
ATOM	680	CG2	ILE	216	15.367	90.029	1.102	1.00	30.52	A
ATOM	681	CG1	ILE	216	15.694	90.973	-1.192	1.00	29.14	A
ATOM	682	CD1	ILE	216	17.084	90.443	-1.481	1.00	27.72	A
ATOM	683	C	ILE	216	13.987	92.335	1.952	1.00	31.56	A
ATOM	684	O	ILE	216	14.823	92.918	2.637	1.00	31.71	A
ATOM	685	N	GLY	217	12.874	91.824	2.458	1.00	33.70	A
ATOM	686	H	GLY	217	12.242	91.354	1.875	1.00	0.00	A
ATOM	687	CA	GLY	217	12.595	91.962	3.872	1.00	36.08	A
ATOM	688	C	GLY	217	13.014	90.749	4.680	1.00	38.70	A
ATOM	689	O	GLY	217	13.112	89.642	4.141	1.00	38.11	A
ATOM	690	N	ARG	218	13.269	90.965	5.968	1.00	37.58	A
ATOM	691	H	ARG	218	13.193	91.876	6.318	1.00	0.00	A
ATOM	692	CA	ARG	218	13.667	89.895	6.884	1.00	38.94	A
ATOM	693	CB	ARG	218	13.990	90.473	8.267	1.00	37.57	A
ATOM	694	CG	ARG	218	14.512	89.462	9.295	1.00	40.84	A
ATOM	695	CD	ARG	218	15.880	89.885	9.830	1.00	43.84	A
ATOM	696	NE	ARG	218	16.011	89.820	11.283	1.00	35.18	A
ATOM	697	HE	ARG	218	16.023	88.935	11.701	1.00	0.00	A
ATOM	698	CZ	ARG	218	16.126	90.882	12.073	1.00	36.87	A
ATOM	699	NH1	ARG	218	16.126	92.114	11.573	1.00	27.19	A
ATOM	700	HH11	ARG	218	16.055	92.253	10.583	1.00	0.00	A
ATOM	701	HH12	ARG	218	16.212	92.903	12.181	1.00	0.00	A
ATOM	702	NH2	ARG	218	16.263	90.706	13.374	1.00	41.63	A
ATOM	703	HH21	ARG	218	16.287	89.785	13.753	1.00	0.00	A
ATOM	704	HH22	ARG	218	16.345	91.499	13.979	1.00	0.00	A
ATOM	705	C	ARG	218	12.546	88.873	7.006	1.00	35.63	A
ATOM	706	O	ARG	218	11.488	89.167	7.556	1.00	43.27	A
ATOM	707	N	GLN	219	12.788	87.667	6.504	1.00	39.56	A
ATOM	708	H	GLN	219	13.661	87.489	6.097	1.00	0.00	A
ATOM	709	CA	GLN	219	11.792	86.602	6.541	1.00	38.70	A
ATOM	710	CB	GLN	219	12.265	85.411	5.694	1.00	33.61	A
ATOM	711	CG	GLN	219	12.960	84.295	6.452	1.00	32.85	A
ATOM	712	CD	GLN	219	12.950	82.995	5.682	1.00	33.39	A
ATOM	713	OE1	GLN	219	12.946	82.990	4.449	1.00	38.03	A
ATOM	714	NE2	GLN	219	12.938	81.883	6.402	1.00	39.97	A
ATOM	715	HE21	GLN	219	12.936	81.933	7.380	1.00	0.00	A
ATOM	716	HE22	GLN	219	12.931	81.032	5.917	1.00	0.00	A
ATOM	717	C	GLN	219	11.465	86.161	7.961	1.00	41.40	A
ATOM	718	O	GLN	219	10.317	85.831	8.269	1.00	40.86	A
ATOM	719	N	GLY	220	12.470	86.161	8.828	1.00	40.86	A
ATOM	720	H	GLY	220	13.369	86.424	8.536	1.00	0.00	A
ATOM	721	CA	GLY	220	12.241	85.771	10.206	1.00	40.81	A
ATOM	722	C	GLY	220	12.464	84.299	10.470	1.00	41.52	A
ATOM	723	O	GLY	220	12.137	83.447	9.650	1.00	37.96	A
ATOM	724	N	GLY	221	13.022	84.001	11.634	1.00	44.63	A
ATOM	725	H	GLY	221	13.258	84.716	12.260	1.00	0.00	A
ATOM	726	CA	GLY	221	13.282	82.623	11.987	1.00	43.63	A
ATOM	727	C	GLY	221	13.912	82.468	13.354	1.00	44.55	A
ATOM	728	O	GLY	221	14.805	83.221	13.742	1.00	40.07	A
ATOM	729	N	LEU	222	13.416	81.477	14.085	1.00	45.22	A
ATOM	730	H	LEU	222	12.691	80.940	13.711	1.00	0.00	A
ATOM	731	CA	LEU	222	13.903	81.151	15.411	1.00	47.35	A
ATOM	732	CB	LEU	222	12.781	80.471	16.207	1.00	54.79	A
ATOM	733	CG	LEU	222	11.395	80.687	15.579	0.01	54.77	A
ATOM	734	CD1	LEU	222	10.343	79.881	16.311	0.01	55.93	A
ATOM	735	CD2	LEU	222	11.048	82.171	15.608	0.01	57.10	A
ATOM	736	C	LEU	222	15.066	80.194	15.172	1.00	47.02	A
ATOM	737	O	LEU	222	16.135	80.340	15.757	1.00	47.47	A
ATOM	738	N	GLN	223	14.837	79.233	14.279	1.00	42.82	A

ATOM	739	H	GLN	223	13.955	79.189	13.857	1.00	0.00	A
ATOM	740	CA	GLN	223	15.837	78.241	13.903	1.00	40.39	A
ATOM	741	CB	GLN	223	15.159	76.915	13.533	1.00	38.83	A
ATOM	742	CG	GLN	223	14.256	76.346	14.617	0.01	40.23	A
ATOM	743	CD	GLN	223	13.344	75.250	14.099	0.01	40.15	A
ATOM	744	OE1	GLN	223	13.163	74.219	14.747	0.01	39.83	A
ATOM	745	NE2	GLN	223	12.765	75.470	12.924	0.01	39.93	A
ATOM	746	HE21	GLN	223	12.935	76.302	12.443	1.00	0.00	A
ATOM	747	HE22	GLN	223	12.171	74.771	12.577	1.00	0.00	A
ATOM	748	C	GLN	223	16.666	78.746	12.713	1.00	40.39	A
ATOM	749	O	GLN	223	16.144	79.404	11.804	1.00	38.90	A
ATOM	750	N	THR	224	17.954	78.413	12.722	1.00	32.13	A
ATOM	751	H	THR	224	18.293	77.864	13.458	1.00	0.00	A
ATOM	752	CA	THR	224	18.885	78.836	11.675	1.00	29.74	A
ATOM	753	CB	THR	224	20.006	79.688	12.333	1.00	28.84	A
ATOM	754	OG1	THR	224	19.462	80.968	12.668	1.00	31.13	A
ATOM	755	HG1	THR	224	19.146	81.401	11.872	1.00	0.00	A
ATOM	756	CG2	THR	224	21.205	79.867	11.415	1.00	24.03	A
ATOM	757	C	THR	224	19.450	77.608	10.940	1.00	25.16	A
ATOM	758	O	THR	224	20.438	77.013	11.366	1.00	21.68	A
ATOM	759	N	MET	225	18.809	77.231	9.837	1.00	23.33	A
ATOM	760	H	MET	225	18.044	77.757	9.525	1.00	0.00	A
ATOM	761	CA	MET	225	19.219	76.051	9.082	1.00	25.92	A
ATOM	762	CB	MET	225	17.979	75.377	8.504	1.00	26.36	A
ATOM	763	CG	MET	225	16.851	75.275	9.495	1.00	24.17	A
ATOM	764	SD	MET	225	17.187	73.904	10.572	1.00	33.11	A
ATOM	765	CE	MET	225	16.928	72.552	9.456	1.00	31.18	A
ATOM	766	C	MET	225	20.205	76.326	7.958	1.00	26.44	A
ATOM	767	O	MET	225	19.850	76.238	6.785	1.00	27.44	A
ATOM	768	N	THR	226	21.446	76.640	8.303	1.00	27.96	A
ATOM	769	H	THR	226	21.699	76.679	9.248	1.00	0.00	A
ATOM	770	CA	THR	226	22.433	76.930	7.268	1.00	26.56	A
ATOM	771	CB	THR	226	23.761	77.426	7.879	1.00	28.59	A
ATOM	772	OG1	THR	226	23.478	78.382	8.904	1.00	29.78	A
ATOM	773	HG1	THR	226	24.301	78.693	9.288	1.00	0.00	A
ATOM	774	CG2	THR	226	24.622	78.102	6.807	1.00	25.78	A
ATOM	775	C	THR	226	22.709	75.740	6.347	1.00	24.98	A
ATOM	776	O	THR	226	22.912	75.922	5.152	1.00	20.19	A
ATOM	777	N	ALA	227	22.709	74.525	6.889	1.00	25.81	A
ATOM	778	H	ALA	227	22.547	74.412	7.848	1.00	0.00	A
ATOM	779	CA	ALA	227	22.953	73.357	6.047	1.00	23.49	A
ATOM	780	CB	ALA	227	22.972	72.077	6.876	1.00	23.86	A
ATOM	781	C	ALA	227	21.851	73.301	4.999	1.00	25.42	A
ATOM	782	O	ALA	227	22.120	73.101	3.815	1.00	26.01	A
ATOM	783	N	LEU	228	20.614	73.503	5.436	1.00	24.83	A
ATOM	784	H	LEU	228	20.464	73.658	6.393	1.00	0.00	A
ATOM	785	CA	LEU	228	19.470	73.499	4.527	1.00	25.07	A
ATOM	786	CB	LEU	228	18.167	73.656	5.305	1.00	22.51	A
ATOM	787	CG	LEU	228	16.898	73.513	4.450	1.00	34.21	A
ATOM	788	CD1	LEU	228	16.775	72.087	3.969	1.00	32.33	A
ATOM	789	CD2	LEU	228	15.667	73.911	5.256	1.00	31.46	A
ATOM	790	C	LEU	228	19.547	74.603	3.464	1.00	23.01	A
ATOM	791	O	LEU	228	19.219	74.373	2.300	1.00	26.47	A
ATOM	792	N	GLY	229	19.960	75.803	3.858	1.00	20.11	A
ATOM	793	H	GLY	229	20.204	75.955	4.796	1.00	0.00	A
ATOM	794	CA	GLY	229	20.050	76.890	2.897	1.00	22.39	A
ATOM	795	C	GLY	229	21.123	76.627	1.852	1.00	25.88	A
ATOM	796	O	GLY	229	20.865	76.706	0.658	1.00	25.69	A
ATOM	797	N	THR	230	22.337	76.313	2.305	1.00	23.82	A
ATOM	798	H	THR	230	22.491	76.274	3.271	1.00	0.00	A
ATOM	799	CA	THR	230	23.441	76.032	1.393	1.00	25.70	A
ATOM	800	CB	THR	230	24.729	75.710	2.182	1.00	25.52	A
ATOM	801	OG1	THR	230	25.233	76.918	2.768	1.00	27.54	A
ATOM	802	HG1	THR	230	26.034	76.726	3.261	1.00	0.00	A
ATOM	803	CG2	THR	230	25.794	75.102	1.266	1.00	18.19	A
ATOM	804	C	THR	230	23.148	74.879	0.424	1.00	26.69	A
ATOM	805	O	THR	230	23.467	74.964	-0.771	1.00	24.80	A
ATOM	806	N	ASP	231	22.525	73.820	0.938	1.00	25.10	A
ATOM	807	H	ASP	231	22.272	73.835	1.884	1.00	0.00	A
ATOM	808	CA	ASP	231	22.203	72.630	0.137	1.00	22.95	A
ATOM	809	CB	ASP	231	21.702	71.504	1.050	1.00	14.71	A
ATOM	810	CG	ASP	231	21.903	70.115	0.444	1.00	26.88	A
ATOM	811	OD1	ASP	231	22.234	70.004	-0.755	1.00	25.70	A

ATOM	812	OD2	ASP	231	21.722	69.124	1.183	1.00	32.43	A
ATOM	813	C	ASP	231	21.149	72.943	-0.900	1.00	25.92	A
ATOM	814	O	ASP	231	21.167	72.412	-2.019	1.00	22.17	A
ATOM	815	N	THR	232	20.216	73.803	-0.513	1.00	30.41	A
ATOM	816	H	THR	232	20.257	74.169	0.395	1.00	0.00	A
ATOM	817	CA	THR	232	19.138	74.216	-1.391	1.00	27.31	A
ATOM	818	CB	THR	232	18.059	74.977	-0.578	1.00	31.03	A
ATOM	819	OG1	THR	232	17.404	74.051	0.299	1.00	30.78	A
ATOM	820	HG1	THR	232	16.732	74.513	0.807	1.00	0.00	A
ATOM	821	CG2	THR	232	17.023	75.618	-1.497	1.00	22.38	A
ATOM	822	C	THR	232	19.716	75.095	-2.502	1.00	27.81	A
ATOM	823	O	THR	232	19.325	74.978	-3.659	1.00	27.44	A
ATOM	824	N	ALA	233	20.676	75.946	-2.148	1.00	27.86	A
ATOM	825	H	ALA	233	20.957	75.979	-1.210	1.00	0.00	A
ATOM	826	CA	ALA	233	21.321	76.830	-3.112	1.00	31.80	A
ATOM	827	CB	ALA	233	22.162	77.876	-2.381	1.00	27.63	A
ATOM	828	C	ALA	233	22.195	76.042	-4.095	1.00	35.25	A
ATOM	829	O	ALA	233	22.341	76.431	-5.255	1.00	37.14	A
ATOM	830	N	ALA	234	22.776	74.940	-3.632	1.00	35.16	A
ATOM	831	H	ALA	234	22.638	74.681	-2.696	1.00	0.00	A
ATOM	832	CA	ALA	234	23.613	74.111	-4.486	1.00	37.73	A
ATOM	833	CB	ALA	234	24.552	73.271	-3.651	1.00	41.51	A
ATOM	834	C	ALA	234	22.712	73.205	-5.293	1.00	40.15	A
ATOM	835	O	ALA	234	23.045	72.806	-6.407	1.00	40.08	A
ATOM	836	N	LYS	235	21.556	72.897	-4.719	1.00	38.44	A
ATOM	837	H	LYS	235	21.342	73.275	-3.841	1.00	0.00	A
ATOM	838	CA	LYS	235	20.601	72.013	-5.361	1.00	37.80	A
ATOM	839	CB	LYS	235	19.826	71.223	-4.299	1.00	39.04	A
ATOM	840	CG	LYS	235	20.401	69.856	-3.977	1.00	40.19	A
ATOM	841	CD	LYS	235	19.542	69.129	-2.957	1.00	40.24	A
ATOM	842	CE	LYS	235	19.458	67.642	-3.268	1.00	40.62	A
ATOM	843	NZ	LYS	235	18.951	66.862	-2.102	1.00	39.60	A
ATOM	844	HZ1	LYS	235	17.999	67.200	-1.848	1.00	0.00	A
ATOM	845	HZ2	LYS	235	19.591	66.994	-1.293	1.00	0.00	A
ATOM	846	HZ3	LYS	235	18.907	65.855	-2.351	1.00	0.00	A
ATOM	847	C	LYS	235	19.605	72.732	-6.253	1.00	37.03	A
ATOM	848	O	LYS	235	19.199	72.193	-7.282	1.00	37.66	A
ATOM	849	N	GLU	236	19.217	73.947	-5.873	1.00	36.11	A
ATOM	850	H	GLU	236	19.615	74.355	-5.080	1.00	0.00	A
ATOM	851	CA	GLU	236	18.210	74.677	-6.640	1.00	39.41	A
ATOM	852	CB	GLU	236	17.025	75.022	-5.736	1.00	40.91	A
ATOM	853	CG	GLU	236	16.053	73.874	-5.542	1.00	47.24	A
ATOM	854	CD	GLU	236	15.185	74.050	-4.312	1.00	50.19	A
ATOM	855	OE1	GLU	236	14.414	75.033	-4.259	1.00	51.54	A
ATOM	856	OE2	GLU	236	15.274	73.203	-3.399	1.00	49.31	A
ATOM	857	C	GLU	236	18.650	75.934	-7.361	1.00	37.57	A
ATOM	858	O	GLU	236	18.484	76.043	-8.574	1.00	39.16	A
ATOM	859	N	ALA	237	19.182	76.893	-6.611	1.00	36.70	A
ATOM	860	H	ALA	237	19.280	76.749	-5.646	1.00	0.00	A
ATOM	861	CA	ALA	237	19.622	78.153	-7.197	1.00	33.79	A
ATOM	862	CB	ALA	237	20.292	79.031	-6.125	1.00	22.28	A
ATOM	863	C	ALA	237	20.586	77.906	-8.357	1.00	31.23	A
ATOM	864	O	ALA	237	20.550	78.610	-9.363	1.00	29.31	A
ATOM	865	N	PHE	238	21.433	76.889	-8.208	1.00	33.83	A
ATOM	866	H	PHE	238	21.384	76.354	-7.391	1.00	0.00	A
ATOM	867	CA	PHE	238	22.428	76.545	-9.220	1.00	33.21	A
ATOM	868	CB	PHE	238	23.691	75.985	-8.558	1.00	33.12	A
ATOM	869	CG	PHE	238	24.552	77.026	-7.908	1.00	33.07	A
ATOM	870	CD1	PHE	238	25.030	76.834	-6.616	1.00	32.77	A
ATOM	871	CD2	PHE	238	24.882	78.195	-8.580	1.00	29.14	A
ATOM	872	CE1	PHE	238	25.821	77.792	-5.999	1.00	29.30	A
ATOM	873	CE2	PHE	238	25.672	79.158	-7.976	1.00	36.10	A
ATOM	874	CZ	PHE	238	26.146	78.957	-6.676	1.00	37.20	A
ATOM	875	C	PHE	238	21.934	75.531	-10.233	1.00	35.57	A
ATOM	876	O	PHE	238	22.487	74.447	-10.347	1.00	34.78	A
ATOM	877	N	THR	239	20.894	75.880	-10.971	1.00	41.07	A
ATOM	878	H	THR	239	20.472	76.755	-10.834	1.00	0.00	A
ATOM	879	CA	THR	239	20.370	74.980	-11.984	1.00	46.32	A
ATOM	880	CB	THR	239	19.073	74.286	-11.508	1.00	46.28	A
ATOM	881	OG1	THR	239	18.000	75.229	-11.474	1.00	46.22	A
ATOM	882	HG1	THR	239	17.861	75.589	-12.353	1.00	0.00	A
ATOM	883	CG2	THR	239	19.272	73.705	-10.116	1.00	51.02	A
ATOM	884	C	THR	239	20.107	75.780	-13.248	1.00	45.38	A

```
ATOM    885  O   THR   239      19.735  76.951 -13.185  1.00 46.02      A
ATOM    886  N   GLU   240      20.320  75.152 -14.396  1.00 48.01      A
ATOM    887  H   GLU   240      20.614  74.216 -14.386  1.00  0.00      A
ATOM    888  CA  GLU   240      20.123  75.825 -15.667  1.00 47.10      A
ATOM    889  CB  GLU   240      20.289  74.833 -16.813  1.00 49.28      A
ATOM    890  CG  GLU   240      21.543  73.981 -16.702  1.00 56.94      A
ATOM    891  CD  GLU   240      22.735  74.606 -17.398  1.00 60.51      A
ATOM    892  OE1 GLU   240      23.662  75.079 -16.700  1.00 61.18      A
ATOM    893  OE2 GLU   240      22.741  74.625 -18.645  1.00 63.05      A
ATOM    894  C   GLU   240      18.737  76.427 -15.691  1.00 48.10      A
ATOM    895  O   GLU   240      18.482  77.397 -16.397  1.00 49.86      A
ATOM    896  N   ALA   241      17.848  75.844 -14.893  1.00 50.22      A
ATOM    897  H   ALA   241      18.132  75.082 -14.346  1.00  0.00      A
ATOM    898  CA  ALA   241      16.468  76.299 -14.808  1.00 51.00      A
ATOM    899  CB  ALA   241      15.611  75.237 -14.132  1.00 48.14      A
ATOM    900  C   ALA   241      16.376  77.600 -14.036  1.00 49.38      A
ATOM    901  O   ALA   241      15.542  78.453 -14.336  1.00 52.67      A
ATOM    902  N   ARG   242      17.238  77.748 -13.039  1.00 43.01      A
ATOM    903  H   ARG   242      17.889  77.041 -12.853  1.00  0.00      A
ATOM    904  CA  ARG   242      17.226  78.944 -12.221  1.00 40.74      A
ATOM    905  CB  ARG   242      17.408  78.562 -10.744  1.00 34.79      A
ATOM    906  CG  ARG   242      16.493  77.376 -10.317  1.00 30.30      A
ATOM    907  CD  ARG   242      15.817  77.532  -8.931  1.00 29.76      A
ATOM    908  NE  ARG   242      14.782  78.570  -8.877  1.00 33.22      A
ATOM    909  HE  ARG   242      14.958  79.399  -9.365  1.00  0.00      A
ATOM    910  CZ  ARG   242      13.635  78.491  -8.196  1.00 29.10      A
ATOM    911  NH1 ARG   242      13.313  77.413  -7.488  1.00 28.44      A
ATOM    912 HH11 ARG   242      13.952  76.653  -7.416  1.00  0.00      A
ATOM    913 HH12 ARG   242      12.442  77.383  -6.994  1.00  0.00      A
ATOM    914  NH2 ARG   242      12.807  79.524  -8.203  1.00 34.29      A
ATOM    915 HH21 ARG   242      13.057  80.361  -8.690  1.00  0.00      A
ATOM    916 HH22 ARG   242      11.938  79.475  -7.709  1.00  0.00      A
ATOM    917  C   ARG   242      18.277  79.944 -12.681  1.00 46.22      A
ATOM    918  O   ARG   242      18.564  80.913 -11.984  1.00 51.48      A
ATOM    919  N   GLY   243      18.850  79.704 -13.860  1.00 48.36      A
ATOM    920  H   GLY   243      18.612  78.899 -14.365  1.00  0.00      A
ATOM    921  CA  GLY   243      19.832  80.634 -14.398  1.00 45.39      A
ATOM    922  C   GLY   243      21.289  80.231 -14.535  1.00 43.38      A
ATOM    923  O   GLY   243      21.993  80.797 -15.371  1.00 43.70      A
ATOM    924  N   ALA   244      21.750  79.276 -13.731  1.00 41.17      A
ATOM    925  H   ALA   244      21.143  78.857 -13.086  1.00  0.00      A
ATOM    926  CA  ALA   244      23.144  78.838 -13.789  1.00 37.01      A
ATOM    927  CB  ALA   244      23.315  77.543 -13.015  1.00 33.03      A
ATOM    928  C   ALA   244      23.635  78.656 -15.223  1.00 39.91      A
ATOM    929  O   ALA   244      22.941  78.070 -16.054  1.00 37.74      A
ATOM    930  N   ARG   245      24.833  79.159 -15.505  1.00 35.79      A
ATOM    931  H   ARG   245      25.344  79.603 -14.803  1.00  0.00      A
ATOM    932  CA  ARG   245      25.406  79.057 -16.839  1.00 37.22      A
ATOM    933  CB  ARG   245      26.112  80.375 -17.205  1.00 37.87      A
ATOM    934  CG  ARG   245      25.170  81.597 -17.186  1.00 41.05      A
ATOM    935  CD  ARG   245      25.919  82.937 -17.270  1.00 39.75      A
ATOM    936  NE  ARG   245      26.703  83.246 -16.071  1.00 32.46      A
ATOM    937  HE  ARG   245      26.520  82.731 -15.258  1.00  0.00      A
ATOM    938  CZ  ARG   245      27.636  84.192 -16.014  1.00 34.10      A
ATOM    939  NH1 ARG   245      27.911  84.933 -17.085  1.00 32.74      A
ATOM    940 HH11 ARG   245      27.400  84.791 -17.934  1.00  0.00      A
ATOM    941 HH12 ARG   245      28.616  85.640 -17.039  1.00  0.00      A
ATOM    942  NH2 ARG   245      28.304  84.397 -14.887  1.00 31.28      A
ATOM    943 HH21 ARG   245      28.098  83.847 -14.077  1.00  0.00      A
ATOM    944 HH22 ARG   245      29.009  85.102 -14.847  1.00  0.00      A
ATOM    945  C   ARG   245      26.366  77.868 -16.937  1.00 37.43      A
ATOM    946  O   ARG   245      27.190  77.640 -16.053  1.00 32.06      A
ATOM    947  N   ARG   246      26.243  77.120 -18.030  1.00 36.45      A
ATOM    948  H   ARG   246      25.576  77.378 -18.700  1.00  0.00      A
ATOM    949  CA  ARG   246      27.052  75.931 -18.279  1.00 40.85      A
ATOM    950  CB  ARG   246      26.710  75.351 -19.655  1.00 47.81      A
ATOM    951  CG  ARG   246      25.360  74.674 -19.728  1.00 56.42      A
ATOM    952  CD  ARG   246      25.331  73.599 -20.805  1.00 65.18      A
ATOM    953  NE  ARG   246      24.144  72.756 -20.688  1.00 70.92      A
ATOM    954  HE  ARG   246      23.939  72.373 -19.811  1.00  0.00      A
ATOM    955  CZ  ARG   246      23.324  72.473 -21.697  1.00 75.61      A
ATOM    956  NH1 ARG   246      22.267  71.694 -21.494  1.00 75.32      A
ATOM    957 HH11 ARG   246      22.087  71.323 -20.583  1.00  0.00      A
```

ATOM	958	HH12	ARG	246	21.650	71.482	-22.252	1.00	0.00	A
ATOM	959	NH2	ARG	246	23.561	72.966	-22.908	1.00	76.75	A
ATOM	960	HH21	ARG	246	24.357	73.550	-23.064	1.00	0.00	A
ATOM	961	HH22	ARG	246	22.943	72.750	-23.664	1.00	0.00	A
ATOM	962	C	ARG	246	28.557	76.143	-18.200	1.00	37.90	A
ATOM	963	O	ARG	246	29.149	76.779	-19.074	1.00	41.30	A
ATOM	964	N	GLY	247	29.172	75.602	-17.157	1.00	30.93	A
ATOM	965	H	GLY	247	28.658	75.119	-16.478	1.00	0.00	A
ATOM	966	CA	GLY	247	30.610	75.728	-17.019	1.00	33.39	A
ATOM	967	C	GLY	247	31.104	77.062	-16.515	1.00	34.40	A
ATOM	968	O	GLY	247	32.280	77.394	-16.648	1.00	37.30	A
ATOM	969	N	VAL	248	30.206	77.853	-15.947	1.00	37.33	A
ATOM	970	H	VAL	248	29.266	77.576	-15.906	1.00	0.00	A
ATOM	971	CA	VAL	248	30.617	79.126	-15.390	1.00	33.83	A
ATOM	972	CB	VAL	248	29.506	80.168	-15.526	1.00	29.27	A
ATOM	973	CG1	VAL	248	29.660	81.239	-14.471	1.00	27.00	A
ATOM	974	CG2	VAL	248	29.559	80.764	-16.916	1.00	18.63	A
ATOM	975	C	VAL	248	30.905	78.819	-13.926	1.00	38.78	A
ATOM	976	O	VAL	248	30.175	78.050	-13.296	1.00	44.51	A
ATOM	977	N	LYS	249	31.985	79.384	-13.397	1.00	37.56	A
ATOM	978	H	LYS	249	32.536	79.980	-13.946	1.00	0.00	A
ATOM	979	CA	LYS	249	32.362	79.135	-12.012	1.00	39.22	A
ATOM	980	CB	LYS	249	33.644	79.894	-11.660	1.00	42.55	A
ATOM	981	CG	LYS	249	34.192	79.585	-10.262	1.00	49.76	A
ATOM	982	CD	LYS	249	34.281	78.082	-9.992	1.00	50.58	A
ATOM	983	CE	LYS	249	34.354	77.781	-8.498	1.00	53.51	A
ATOM	984	NZ	LYS	249	35.759	77.621	-8.011	1.00	56.75	A
ATOM	985	HZ1	LYS	249	36.289	78.498	-8.188	1.00	0.00	A
ATOM	986	HZ2	LYS	249	36.213	76.834	-8.518	1.00	0.00	A
ATOM	987	HZ3	LYS	249	35.752	77.418	-6.992	1.00	0.00	A
ATOM	988	C	LYS	249	31.250	79.519	-11.045	1.00	37.78	A
ATOM	989	O	LYS	249	30.689	80.614	-11.120	1.00	39.09	A
ATOM	990	N	LYS	250	30.934	78.602	-10.140	1.00	34.03	A
ATOM	991	H	LYS	250	31.418	77.750	-10.132	1.00	0.00	A
ATOM	992	CA	LYS	250	29.888	78.833	-9.161	1.00	33.73	A
ATOM	993	CB	LYS	250	29.116	77.537	-8.890	1.00	32.39	A
ATOM	994	CG	LYS	250	28.185	77.111	-10.006	1.00	30.52	A
ATOM	995	CD	LYS	250	28.424	75.659	-10.376	1.00	33.84	A
ATOM	996	CE	LYS	250	27.324	74.777	-9.831	1.00	33.72	A
ATOM	997	NZ	LYS	250	26.219	74.661	-10.810	1.00	37.02	A
ATOM	998	HZ1	LYS	250	26.577	74.247	-11.692	1.00	0.00	A
ATOM	999	HZ2	LYS	250	25.828	75.607	-11.003	1.00	0.00	A
ATOM	1000	HZ3	LYS	250	25.471	74.054	-10.418	1.00	0.00	A
ATOM	1001	C	LYS	250	30.499	79.326	-7.864	1.00	32.94	A
ATOM	1002	O	LYS	250	31.433	78.718	-7.341	1.00	31.11	A
ATOM	1003	N	VAL	251	29.981	80.441	-7.360	1.00	28.36	A
ATOM	1004	H	VAL	251	29.264	80.901	-7.843	1.00	0.00	A
ATOM	1005	CA	VAL	251	30.461	80.987	-6.105	1.00	29.32	A
ATOM	1006	CB	VAL	251	31.228	82.296	-6.310	1.00	33.68	A
ATOM	1007	CG1	VAL	251	31.611	82.882	-4.965	1.00	30.93	A
ATOM	1008	CG2	VAL	251	32.478	82.030	-7.137	1.00	35.10	A
ATOM	1009	C	VAL	251	29.308	81.236	-5.142	1.00	27.80	A
ATOM	1010	O	VAL	251	28.229	81.672	-5.534	1.00	23.98	A
ATOM	1011	N	MET	252	29.557	80.955	-3.874	1.00	27.02	A
ATOM	1012	H	MET	252	30.442	80.618	-3.628	1.00	0.00	A
ATOM	1013	CA	MET	252	28.562	81.134	-2.841	1.00	29.16	A
ATOM	1014	CB	MET	252	28.251	79.779	-2.192	1.00	31.45	A
ATOM	1015	CG	MET	252	26.775	79.497	-1.946	1.00	32.24	A
ATOM	1016	SD	MET	252	26.458	77.877	-1.174	1.00	36.40	A
ATOM	1017	CE	MET	252	26.088	76.900	-2.663	1.00	27.09	A
ATOM	1018	C	MET	252	29.057	82.114	-1.779	1.00	27.61	A
ATOM	1019	O	MET	252	30.215	82.067	-1.363	1.00	32.25	A
ATOM	1020	N	VAL	253	28.183	83.028	-1.376	1.00	27.62	A
ATOM	1021	H	VAL	253	27.302	83.065	-1.801	1.00	0.00	A
ATOM	1022	CA	VAL	253	28.509	83.981	-0.320	1.00	29.51	A
ATOM	1023	CB	VAL	253	28.518	85.459	-0.821	1.00	26.29	A
ATOM	1024	CG1	VAL	253	28.967	86.368	0.305	1.00	28.02	A
ATOM	1025	CG2	VAL	253	29.446	85.625	-2.024	1.00	23.28	A
ATOM	1026	C	VAL	253	27.414	83.825	0.754	1.00	28.07	A
ATOM	1027	O	VAL	253	26.301	84.333	0.598	1.00	25.71	A
ATOM	1028	N	ILE	254	27.737	83.107	1.828	1.00	29.62	A
ATOM	1029	H	ILE	254	28.635	82.721	1.881	1.00	0.00	A
ATOM	1030	CA	ILE	254	26.808	82.874	2.931	1.00	25.76	A

ATOM	1031	CB	ILE	254	26.933	81.416	3.476	1.00	26.55	A
ATOM	1032	CG2	ILE	254	25.851	81.144	4.512	1.00	23.36	A
ATOM	1033	CG1	ILE	254	26.764	80.415	2.330	1.00	23.69	A
ATOM	1034	CD1	ILE	254	28.047	79.781	1.869	1.00	23.22	A
ATOM	1035	C	ILE	254	27.076	83.879	4.053	1.00	23.27	A
ATOM	1036	O	ILE	254	28.222	84.121	4.418	1.00	26.33	A
ATOM	1037	N	VAL	255	26.000	84.452	4.590	1.00	19.71	A
ATOM	1038	H	VAL	255	25.120	84.171	4.270	1.00	0.00	A
ATOM	1039	CA	VAL	255	26.059	85.474	5.631	1.00	18.36	A
ATOM	1040	CB	VAL	255	25.492	86.818	5.063	1.00	19.62	A
ATOM	1041	CG1	VAL	255	25.599	87.923	6.080	1.00	17.22	A
ATOM	1042	CG2	VAL	255	26.254	87.209	3.790	1.00	20.74	A
ATOM	1043	C	VAL	255	25.220	84.990	6.812	1.00	16.43	A
ATOM	1044	O	VAL	255	24.035	84.701	6.649	1.00	19.58	A
ATOM	1045	N	THR	256	25.826	84.875	7.990	1.00	15.49	A
ATOM	1046	H	THR	256	26.770	85.121	8.082	1.00	0.00	A
ATOM	1047	CA	THR	256	25.084	84.390	9.142	1.00	14.90	A
ATOM	1048	CB	THR	256	25.113	82.858	9.212	1.00	14.75	A
ATOM	1049	OG1	THR	256	24.240	82.400	10.253	1.00	13.11	A
ATOM	1050	HG1	THR	256	24.525	82.758	11.096	1.00	0.00	A
ATOM	1051	CG2	THR	256	26.526	82.378	9.476	1.00	12.09	A
ATOM	1052	C	THR	256	25.501	84.938	10.494	1.00	20.05	A
ATOM	1053	O	THR	256	26.661	85.291	10.724	1.00	16.01	A
ATOM	1054	N	ASP	257	24.512	84.930	11.385	1.00	21.65	A
ATOM	1055	H	ASP	257	23.664	84.542	11.090	1.00	0.00	A
ATOM	1056	CA	ASP	257	24.557	85.440	12.757	1.00	24.04	A
ATOM	1057	CB	ASP	257	23.199	86.096	13.031	1.00	29.68	A
ATOM	1058	CG	ASP	257	23.297	87.308	13.891	1.00	38.27	A
ATOM	1059	OD1	ASP	257	24.426	87.791	14.137	1.00	52.10	A
ATOM	1060	OD2	ASP	257	22.228	87.780	14.321	1.00	36.38	A
ATOM	1061	C	ASP	257	24.831	84.444	13.904	1.00	16.57	A
ATOM	1062	O	ASP	257	25.087	84.859	15.036	1.00	15.92	A
ATOM	1063	N	GLY	258	24.731	83.150	13.643	1.00	12.93	A
ATOM	1064	H	GLY	258	24.516	82.837	12.744	1.00	0.00	A
ATOM	1065	CA	GLY	258	24.950	82.198	14.721	1.00	16.21	A
ATOM	1066	C	GLY	258	25.155	80.786	14.229	1.00	21.42	A
ATOM	1067	O	GLY	258	25.226	80.552	13.026	1.00	16.78	A
ATOM	1068	N	GLU	259	25.254	79.845	15.167	1.00	21.61	A
ATOM	1069	H	GLU	259	25.190	80.105	16.110	1.00	0.00	A
ATOM	1070	CA	GLU	259	25.450	78.442	14.832	1.00	22.54	A
ATOM	1071	CB	GLU	259	25.801	77.649	16.093	1.00	27.50	A
ATOM	1072	CG	GLU	259	26.886	78.305	16.911	1.00	38.06	A
ATOM	1073	CD	GLU	259	27.536	77.361	17.891	1.00	39.46	A
ATOM	1074	OE1	GLU	259	28.417	76.578	17.468	1.00	44.28	A
ATOM	1075	OE2	GLU	259	27.167	77.410	19.083	1.00	40.01	A
ATOM	1076	C	GLU	259	24.196	77.875	14.187	1.00	19.71	A
ATOM	1077	O	GLU	259	23.093	78.316	14.468	1.00	16.96	A
ATOM	1078	N	SER	260	24.357	76.886	13.324	1.00	21.81	A
ATOM	1079	H	SER	260	25.252	76.526	13.145	1.00	0.00	A
ATOM	1080	CA	SER	260	23.197	76.337	12.649	1.00	24.30	A
ATOM	1081	CB	SER	260	23.585	75.761	11.287	1.00	26.30	A
ATOM	1082	OG	SER	260	24.643	74.827	11.404	1.00	27.86	A
ATOM	1083	HG	SER	260	25.412	75.260	11.780	1.00	0.00	A
ATOM	1084	C	SER	260	22.492	75.279	13.456	1.00	24.11	A
ATOM	1085	O	SER	260	23.123	74.488	14.150	1.00	19.93	A
ATOM	1086	N	HIS	261	21.166	75.303	13.384	1.00	30.37	A
ATOM	1087	H	HIS	261	20.726	76.006	12.864	1.00	0.00	A
ATOM	1088	CA	HIS	261	20.352	74.308	14.062	1.00	35.00	A
ATOM	1089	CB	HIS	261	18.862	74.616	13.876	1.00	38.14	A
ATOM	1090	CG	HIS	261	18.263	75.417	14.994	1.00	40.87	A
ATOM	1091	CD2	HIS	261	17.159	75.203	15.749	1.00	38.31	A
ATOM	1092	ND1	HIS	261	18.809	76.600	15.444	1.00	42.06	A
ATOM	1093	HD1	HIS	261	19.620	77.019	15.088	1.00	0.00	A
ATOM	1094	CE1	HIS	261	18.071	77.080	16.425	1.00	41.84	A
ATOM	1095	NE2	HIS	261	17.062	76.251	16.631	1.00	38.37	A
ATOM	1096	HE2	HIS	261	16.358	76.361	17.297	1.00	0.00	A
ATOM	1097	C	HIS	261	20.715	73.032	13.316	1.00	36.08	A
ATOM	1098	O	HIS	261	20.886	71.969	13.915	1.00	32.42	A
ATOM	1099	N	TYR	262	20.857	73.173	11.997	1.00	39.63	A
ATOM	1100	H	TYR	262	20.705	74.056	11.602	1.00	0.00	A
ATOM	1101	CA	TYR	262	21.224	72.069	11.122	1.00	45.92	A
ATOM	1102	CB	TYR	262	20.783	72.372	9.689	1.00	52.25	A
ATOM	1103	CG	TYR	262	19.879	71.310	9.137	1.00	62.19	A

ATOM	1104	CD1	TYR	262	19.511	71.302	7.792	1.00	67.63	A
ATOM	1105	CE1	TYR	262	18.676	70.297	7.280	1.00	69.78	A
ATOM	1106	CD2	TYR	262	19.398	70.290	9.960	1.00	66.65	A
ATOM	1107	CE2	TYR	262	18.569	69.285	9.465	1.00	69.62	A
ATOM	1108	CZ	TYR	262	18.213	69.290	8.125	1.00	71.57	A
ATOM	1109	OH	TYR	262	17.408	68.282	7.637	1.00	70.23	A
ATOM	1110	HH	TYR	262	17.185	67.678	8.350	1.00	0.00	A
ATOM	1111	C	TYR	262	22.728	71.793	11.152	1.00	45.91	A
ATOM	1112	O	TYR	262	23.270	71.219	10.215	1.00	45.20	A
ATOM	1113	N	ASN	263	23.377	72.230	12.233	1.00	47.51	A
ATOM	1114	H	ASN	263	22.849	72.702	12.906	1.00	0.00	A
ATOM	1115	CA	ASN	263	24.817	72.066	12.500	1.00	47.67	A
ATOM	1116	CB	ASN	263	25.022	71.886	14.011	1.00	49.01	A
ATOM	1117	CG	ASN	263	26.334	72.466	14.504	1.00	54.05	A
ATOM	1118	OD1	ASN	263	27.373	71.805	14.449	1.00	54.43	A
ATOM	1119	ND2	ASN	263	26.290	73.702	15.000	1.00	47.01	A
ATOM	1120	HD21	ASN	263	25.440	74.188	15.032	1.00	0.00	A
ATOM	1121	HD22	ASN	263	27.130	74.088	15.322	1.00	0.00	A
ATOM	1122	C	ASN	263	25.434	70.873	11.775	1.00	49.23	A
ATOM	1123	O	ASN	263	26.273	71.026	10.881	1.00	46.48	A
ATOM	1124	N	HIS	264	25.029	69.681	12.197	1.00	48.43	A
ATOM	1125	H	HIS	264	24.391	69.635	12.939	1.00	0.00	A
ATOM	1126	CA	HIS	264	25.496	68.439	11.599	1.00	47.59	A
ATOM	1127	CB	HIS	264	24.755	67.255	12.228	1.00	46.90	A
ATOM	1128	CG	HIS	264	23.275	67.462	12.359	1.00	50.04	A
ATOM	1129	CD2	HIS	264	22.549	68.207	13.229	1.00	53.97	A
ATOM	1130	ND1	HIS	264	22.360	66.865	11.517	1.00	51.14	A
ATOM	1131	HD1	HIS	264	22.581	66.256	10.788	1.00	0.00	A
ATOM	1132	CE1	HIS	264	21.138	67.228	11.864	1.00	53.11	A
ATOM	1133	NE2	HIS	264	21.225	68.044	12.898	1.00	55.29	A
ATOM	1134	HE2	HIS	264	20.471	68.460	13.361	1.00	0.00	A
ATOM	1135	C	HIS	264	25.132	68.550	10.130	1.00	46.97	A
ATOM	1136	O	HIS	264	24.666	69.593	9.686	1.00	51.57	A
ATOM	1137	N	ARG	265	25.348	67.496	9.358	1.00	44.23	A
ATOM	1138	H	ARG	265	25.749	66.684	9.732	1.00	0.00	A
ATOM	1139	CA	ARG	265	24.983	67.554	7.946	1.00	41.47	A
ATOM	1140	CB	ARG	265	23.473	67.816	7.831	1.00	40.64	A
ATOM	1141	CG	ARG	265	23.030	68.564	6.591	1.00	43.80	A
ATOM	1142	CD	ARG	265	21.666	68.091	6.130	1.00	47.91	A
ATOM	1143	NE	ARG	265	21.163	68.876	5.005	1.00	56.53	A
ATOM	1144	HE	ARG	265	21.797	69.449	4.527	1.00	0.00	A
ATOM	1145	CZ	ARG	265	19.901	68.861	4.588	1.00	58.89	A
ATOM	1146	NH1	ARG	265	19.006	68.099	5.202	1.00	64.72	A
ATOM	1147	HH11	ARG	265	19.281	67.532	5.979	1.00	0.00	A
ATOM	1148	HH12	ARG	265	18.057	68.088	4.887	1.00	0.00	A
ATOM	1149	NH2	ARG	265	19.530	69.612	3.561	1.00	63.20	A
ATOM	1150	HH21	ARG	265	20.200	70.192	3.097	1.00	0.00	A
ATOM	1151	HH22	ARG	265	18.580	69.600	3.250	1.00	0.00	A
ATOM	1152	C	ARG	265	25.777	68.622	7.176	1.00	37.16	A
ATOM	1153	O	ARG	265	25.768	68.641	5.943	1.00	37.73	A
ATOM	1154	N	LEU	266	26.466	69.497	7.904	1.00	30.79	A
ATOM	1155	H	LEU	266	26.433	69.434	8.878	1.00	0.00	A
ATOM	1156	CA	LEU	266	27.274	70.551	7.290	1.00	37.31	A
ATOM	1157	CB	LEU	266	27.832	71.482	8.368	1.00	31.59	A
ATOM	1158	CG	LEU	266	27.685	73.002	8.258	1.00	31.43	A
ATOM	1159	CD1	LEU	266	26.593	73.400	7.273	1.00	36.39	A
ATOM	1160	CD2	LEU	266	27.383	73.540	9.638	1.00	28.41	A
ATOM	1161	C	LEU	266	28.430	69.925	6.523	1.00	42.12	A
ATOM	1162	O	LEU	266	28.719	70.299	5.388	1.00	43.04	A
ATOM	1163	N	GLN	267	29.091	68.967	7.164	1.00	46.26	A
ATOM	1164	H	GLN	267	28.809	68.723	8.070	1.00	0.00	A
ATOM	1165	CA	GLN	267	30.218	68.269	6.567	1.00	48.62	A
ATOM	1166	CB	GLN	267	30.721	67.188	7.521	1.00	54.56	A
ATOM	1167	CG	GLN	267	30.666	67.601	8.987	1.00	62.75	A
ATOM	1168	CD	GLN	267	31.869	67.127	9.787	1.00	67.47	A
ATOM	1169	OE1	GLN	267	32.730	66.406	9.273	1.00	71.87	A
ATOM	1170	NE2	GLN	267	31.935	67.527	11.055	1.00	68.16	A
ATOM	1171	HE21	GLN	267	31.227	68.098	11.420	1.00	0.00	A
ATOM	1172	HE22	GLN	267	32.700	67.231	11.584	1.00	0.00	A
ATOM	1173	C	GLN	267	29.830	67.649	5.231	1.00	48.74	A
ATOM	1174	O	GLN	267	30.597	67.700	4.271	1.00	47.96	A
ATOM	1175	N	LYS	268	28.637	67.067	5.166	1.00	45.46	A
ATOM	1176	H	LYS	268	28.058	67.047	5.955	1.00	0.00	A

```
ATOM   1177  CA  LYS   268      28.191  66.463   3.924  1.00 45.48      A
ATOM   1178  CB  LYS   268      27.048  65.477   4.181  1.00 49.81      A
ATOM   1179  CG  LYS   268      27.042  64.279   3.240  1.00 56.67      A
ATOM   1180  CD  LYS   268      28.157  63.290   3.578  1.00 61.88      A
ATOM   1181  CE  LYS   268      29.009  62.946   2.354  1.00 64.81      A
ATOM   1182  NZ  LYS   268      29.927  61.787   2.599  1.00 70.64      A
ATOM   1183  HZ1 LYS   268      29.368  60.945   2.844  1.00  0.00      A
ATOM   1184  HZ2 LYS   268      30.573  62.014   3.383  1.00  0.00      A
ATOM   1185  HZ3 LYS   268      30.482  61.595   1.740  1.00  0.00      A
ATOM   1186  C   LYS   268      27.744  67.533   2.939  1.00 40.50      A
ATOM   1187  O   LYS   268      27.960  67.402   1.742  1.00 40.62      A
ATOM   1188  N   VAL   269      27.133  68.603   3.434  1.00 39.04      A
ATOM   1189  H   VAL   269      26.991  68.684   4.400  1.00  0.00      A
ATOM   1190  CA  VAL   269      26.676  69.663   2.538  1.00 37.29      A
ATOM   1191  CB  VAL   269      25.782  70.685   3.269  1.00 34.20      A
ATOM   1192  CG1 VAL   269      25.492  71.860   2.356  1.00 29.69      A
ATOM   1193  CG2 VAL   269      24.492  70.026   3.703  1.00 31.32      A
ATOM   1194  C   VAL   269      27.857  70.404   1.921  1.00 35.64      A
ATOM   1195  O   VAL   269      27.844  70.725   0.734  1.00 37.28      A
ATOM   1196  N   ILE   270      28.876  70.667   2.731  1.00 31.83      A
ATOM   1197  H   ILE   270      28.833  70.374   3.661  1.00  0.00      A
ATOM   1198  CA  ILE   270      30.052  71.375   2.261  1.00 33.15      A
ATOM   1199  CB  ILE   270      30.971  71.750   3.438  1.00 33.05      A
ATOM   1200  CG2 ILE   270      32.222  72.469   2.930  1.00 24.49      A
ATOM   1201  CG1 ILE   270      30.209  72.643   4.417  1.00 29.68      A
ATOM   1202  CD1 ILE   270      30.041  74.059   3.944  1.00 32.31      A
ATOM   1203  C   ILE   270      30.835  70.541   1.252  1.00 38.00      A
ATOM   1204  O   ILE   270      31.190  71.026   0.176  1.00 34.89      A
ATOM   1205  N   GLN   271      31.092  69.283   1.603  1.00 37.30      A
ATOM   1206  H   GLN   271      30.776  68.956   2.471  1.00  0.00      A
ATOM   1207  CA  GLN   271      31.836  68.378   0.735  1.00 40.28      A
ATOM   1208  CB  GLN   271      32.061  67.038   1.442  1.00 45.96      A
ATOM   1209  CG  GLN   271      32.724  65.972   0.580  1.00 50.37      A
ATOM   1210  CD  GLN   271      34.111  66.365   0.114  1.00 54.51      A
ATOM   1211  OE1 GLN   271      34.298  66.806  -1.026  1.00 54.16      A
ATOM   1212  NE2 GLN   271      35.102  66.201   0.988  1.00 55.62      A
ATOM   1213  HE21 GLN   271      34.908  65.841   1.879  1.00  0.00      A
ATOM   1214  HE22 GLN   271      36.004  66.448   0.704  1.00  0.00      A
ATOM   1215  C   GLN   271      31.103  68.154  -0.583  1.00 42.88      A
ATOM   1216  O   GLN   271      31.722  67.846  -1.599  1.00 46.33      A
ATOM   1217  N   ASP   272      29.783  68.297  -0.566  1.00 40.17      A
ATOM   1218  H   ASP   272      29.330  68.520   0.276  1.00  0.00      A
ATOM   1219  CA  ASP   272      28.999  68.125  -1.778  1.00 41.34      A
ATOM   1220  CB  ASP   272      27.529  67.885  -1.439  1.00 43.85      A
ATOM   1221  CG  ASP   272      27.249  66.451  -1.068  1.00 45.57      A
ATOM   1222  OD1 ASP   272      27.395  66.103   0.115  1.00 46.69      A
ATOM   1223  OD2 ASP   272      26.885  65.663  -1.960  1.00 53.57      A
ATOM   1224  C   ASP   272      29.128  69.379  -2.632  1.00 41.62      A
ATOM   1225  O   ASP   272      28.871  69.354  -3.841  1.00 39.28      A
ATOM   1226  N   CYS   273      29.520  70.477  -1.992  1.00 37.21      A
ATOM   1227  H   CYS   273      29.694  70.431  -1.028  1.00  0.00      A
ATOM   1228  CA  CYS   273      29.697  71.746  -2.685  1.00 34.88      A
ATOM   1229  CB  CYS   273      29.580  72.910  -1.697  1.00 28.59      A
ATOM   1230  SG  CYS   273      27.871  73.342  -1.278  1.00 31.88      A
ATOM   1231  C   CYS   273      31.078  71.760  -3.326  1.00 34.92      A
ATOM   1232  O   CYS   273      31.226  72.094  -4.504  1.00 26.50      A
ATOM   1233  N   GLU   274      32.072  71.384  -2.524  1.00 35.57      A
ATOM   1234  H   GLU   274      31.847  71.129  -1.606  1.00  0.00      A
ATOM   1235  CA  GLU   274      33.470  71.329  -2.924  1.00 38.47      A
ATOM   1236  CB  GLU   274      34.305  70.927  -1.706  1.00 45.16      A
ATOM   1237  CG  GLU   274      35.785  70.680  -1.935  1.00 50.75      A
ATOM   1238  CD  GLU   274      36.356  69.705  -0.908  1.00 56.66      A
ATOM   1239  OE1 GLU   274      37.306  70.063  -0.173  1.00 58.10      A
ATOM   1240  OE2 GLU   274      35.846  68.569  -0.833  1.00 62.18      A
ATOM   1241  C   GLU   274      33.629  70.318  -4.054  1.00 43.44      A
ATOM   1242  O   GLU   274      34.555  70.407  -4.862  1.00 46.62      A
ATOM   1243  N   ASP   275      32.713  69.357  -4.112  1.00 44.68      A
ATOM   1244  H   ASP   275      32.002  69.326  -3.440  1.00  0.00      A
ATOM   1245  CA  ASP   275      32.757  68.356  -5.160  1.00 43.67      A
ATOM   1246  CB  ASP   275      31.995  67.104  -4.737  1.00 48.36      A
ATOM   1247  CG  ASP   275      32.919  65.936  -4.468  1.00 49.82      A
ATOM   1248  OD1 ASP   275      32.936  64.992  -5.286  1.00 54.38      A
ATOM   1249  OD2 ASP   275      33.634  65.969  -3.443  1.00 54.23      A
```

```
ATOM   1250  C   ASP  275      32.158  68.947  -6.428  1.00 43.28      A
ATOM   1251  O   ASP  275      32.578  68.610  -7.540  1.00 35.41      A
ATOM   1252  N   GLU  276      31.187  69.840  -6.256  1.00 39.61      A
ATOM   1253  H   GLU  276      30.890  70.058  -5.349  1.00  0.00      A
ATOM   1254  CA  GLU  276      30.551  70.503  -7.392  1.00 42.30      A
ATOM   1255  CB  GLU  276      29.085  70.815  -7.078  1.00 44.73      A
ATOM   1256  CG  GLU  276      28.246  69.581  -6.784  1.00 47.48      A
ATOM   1257  CD  GLU  276      26.769  69.817  -7.011  1.00 50.24      A
ATOM   1258  OE1 GLU  276      25.950  69.064  -6.437  1.00 50.57      A
ATOM   1259  OE2 GLU  276      26.428  70.755  -7.762  1.00 48.92      A
ATOM   1260  C   GLU  276      31.314  71.793  -7.678  1.00 40.70      A
ATOM   1261  O   GLU  276      30.789  72.716  -8.301  1.00 40.89      A
ATOM   1262  N   ASN  277      32.563  71.829  -7.211  1.00 40.17      A
ATOM   1263  H   ASN  277      32.899  71.045  -6.732  1.00  0.00      A
ATOM   1264  CA  ASN  277      33.465  72.974  -7.373  1.00 40.38      A
ATOM   1265  CB  ASN  277      34.157  72.914  -8.733  1.00 41.95      A
ATOM   1266  CG  ASN  277      35.220  71.832  -8.789  1.00 47.84      A
ATOM   1267  OD1 ASN  277      36.408  72.097  -8.578  1.00 49.04      A
ATOM   1268  ND2 ASN  277      34.791  70.605  -9.066  1.00 46.30      A
ATOM   1269  HD21 ASN  277      33.840  70.438  -9.221  1.00  0.00      A
ATOM   1270  HD22 ASN  277      35.466  69.895  -9.104  1.00  0.00      A
ATOM   1271  C   ASN  277      32.791  74.327  -7.192  1.00 36.39      A
ATOM   1272  O   ASN  277      32.712  75.137  -8.119  1.00 36.27      A
ATOM   1273  N   ILE  278      32.320  74.569  -5.980  1.00 34.58      A
ATOM   1274  H   ILE  278      32.422  73.890  -5.281  1.00  0.00      A
ATOM   1275  CA  ILE  278      31.652  75.819  -5.665  1.00 34.26      A
ATOM   1276  CB  ILE  278      30.228  75.549  -5.162  1.00 30.91      A
ATOM   1277  CG2 ILE  278      29.646  76.814  -4.530  1.00 32.30      A
ATOM   1278  CG1 ILE  278      29.368  75.058  -6.331  1.00 26.81      A
ATOM   1279  CD1 ILE  278      27.955  74.622  -5.936  1.00 27.38      A
ATOM   1280  C   ILE  278      32.424  76.617  -4.616  1.00 35.39      A
ATOM   1281  O   ILE  278      32.412  76.275  -3.431  1.00 35.14      A
ATOM   1282  N   GLN  279      33.105  77.671  -5.062  1.00 34.70      A
ATOM   1283  H   GLN  279      33.095  77.872  -6.022  1.00  0.00      A
ATOM   1284  CA  GLN  279      33.869  78.537  -4.166  1.00 33.01      A
ATOM   1285  CB  GLN  279      34.560  79.647  -4.954  1.00 38.07      A
ATOM   1286  CG  GLN  279      35.956  79.282  -5.430  1.00 46.02      A
ATOM   1287  CD  GLN  279      37.019  80.222  -4.886  1.00 49.56      A
ATOM   1288  OE1 GLN  279      36.779  81.422  -4.726  1.00 40.91      A
ATOM   1289  NE2 GLN  279      38.205  79.680  -4.601  1.00 48.01      A
ATOM   1290  HE21 GLN  279      38.352  78.722  -4.749  1.00  0.00      A
ATOM   1291  HE22 GLN  279      38.901  80.273  -4.252  1.00  0.00      A
ATOM   1292  C   GLN  279      32.900  79.155  -3.163  1.00 30.48      A
ATOM   1293  O   GLN  279      31.861  79.680  -3.543  1.00 26.66      A
ATOM   1294  N   ARG  280      33.253  79.098  -1.882  1.00 31.39      A
ATOM   1295  H   ARG  280      34.114  78.698  -1.641  1.00  0.00      A
ATOM   1296  CA  ARG  280      32.388  79.622  -0.833  1.00 32.62      A
ATOM   1297  CB  ARG  280      31.864  78.452   0.013  1.00 31.05      A
ATOM   1298  CG  ARG  280      31.447  77.246  -0.823  1.00 30.23      A
ATOM   1299  CD  ARG  280      31.031  76.072   0.033  1.00 29.02      A
ATOM   1300  NE  ARG  280      32.172  75.403   0.641  1.00 23.82      A
ATOM   1301  HE  ARG  280      32.358  75.574   1.588  1.00  0.00      A
ATOM   1302  CZ  ARG  280      32.972  74.567  -0.008  1.00 30.22      A
ATOM   1303  NH1 ARG  280      32.756  74.297  -1.290  1.00 32.10      A
ATOM   1304  HH11 ARG  280      31.983  74.717  -1.766  1.00  0.00      A
ATOM   1305  HH12 ARG  280      33.362  73.669  -1.778  1.00  0.00      A
ATOM   1306  NH2 ARG  280      33.985  73.996   0.627  1.00 33.41      A
ATOM   1307  HH21 ARG  280      34.141  74.190   1.595  1.00  0.00      A
ATOM   1308  HH22 ARG  280      34.592  73.369   0.138  1.00  0.00      A
ATOM   1309  C   ARG  280      33.046  80.673   0.070  1.00 31.10      A
ATOM   1310  O   ARG  280      34.146  80.477   0.598  1.00 29.04      A
ATOM   1311  N   PHE  281      32.354  81.792   0.231  1.00 27.75      A
ATOM   1312  H   PHE  281      31.499  81.890  -0.231  1.00  0.00      A
ATOM   1313  CA  PHE  281      32.824  82.879   1.074  1.00 30.07      A
ATOM   1314  CB  PHE  281      32.798  84.199   0.303  1.00 28.77      A
ATOM   1315  CG  PHE  281      33.920  84.348  -0.671  1.00 31.37      A
ATOM   1316  CD1 PHE  281      33.774  83.928  -1.988  1.00 37.93      A
ATOM   1317  CD2 PHE  281      35.136  84.893  -0.272  1.00 33.95      A
ATOM   1318  CE1 PHE  281      34.830  84.047  -2.894  1.00 38.18      A
ATOM   1319  CE2 PHE  281      36.196  85.014  -1.174  1.00 31.36      A
ATOM   1320  CZ  PHE  281      36.042  84.591  -2.481  1.00 33.33      A
ATOM   1321  C   PHE  281      31.857  82.952   2.247  1.00 31.00      A
ATOM   1322  O   PHE  281      30.676  83.214   2.045  1.00 33.33      A
```

ATOM	1323	N	SER	282	32.337	82.708	3.463	1.00	27.38	A
ATOM	1324	H	SER	282	33.286	82.493	3.582	1.00	0.00	A
ATOM	1325	CA	SER	282	31.455	82.765	4.610	1.00	31.18	A
ATOM	1326	CB	SER	282	31.462	81.425	5.359	1.00	29.23	A
ATOM	1327	OG	SER	282	32.690	81.189	6.020	1.00	25.15	A
ATOM	1328	HG	SER	282	33.402	81.171	5.376	1.00	0.00	A
ATOM	1329	C	SER	282	31.777	83.919	5.560	1.00	32.76	A
ATOM	1330	O	SER	282	32.886	84.044	6.079	1.00	37.88	A
ATOM	1331	N	ILE	283	30.777	84.766	5.766	1.00	33.62	A
ATOM	1332	H	ILE	283	29.927	84.603	5.308	1.00	0.00	A
ATOM	1333	CA	ILE	283	30.887	85.921	6.634	1.00	30.37	A
ATOM	1334	CB	ILE	283	30.324	87.183	5.944	1.00	33.69	A
ATOM	1335	CG2	ILE	283	30.920	88.435	6.571	1.00	33.06	A
ATOM	1336	CG1	ILE	283	30.634	87.144	4.448	1.00	28.09	A
ATOM	1337	CD1	ILE	283	30.588	88.512	3.781	1.00	33.55	A
ATOM	1338	C	ILE	283	30.095	85.671	7.911	1.00	30.75	A
ATOM	1339	O	ILE	283	28.878	85.485	7.869	1.00	30.38	A
ATOM	1340	N	ALA	284	30.797	85.658	9.038	1.00	25.22	A
ATOM	1341	H	ALA	284	31.767	85.785	8.990	1.00	0.00	A
ATOM	1342	CA	ALA	284	30.183	85.462	10.344	1.00	25.92	A
ATOM	1343	CB	ALA	284	31.034	84.480	11.172	1.00	26.80	A
ATOM	1344	C	ALA	284	30.026	86.790	11.114	1.00	25.45	A
ATOM	1345	O	ALA	284	31.025	87.437	11.458	1.00	23.52	A
ATOM	1346	N	ILE	285	28.780	87.188	11.379	1.00	21.71	A
ATOM	1347	H	ILE	285	28.033	86.646	11.052	1.00	0.00	A
ATOM	1348	CA	ILE	285	28.484	88.404	12.142	1.00	14.56	A
ATOM	1349	CB	ILE	285	27.122	89.033	11.672	1.00	20.57	A
ATOM	1350	CG2	ILE	285	26.861	90.366	12.360	1.00	16.36	A
ATOM	1351	CG1	ILE	285	27.157	89.301	10.171	1.00	15.00	A
ATOM	1352	CD1	ILE	285	25.781	89.470	9.533	1.00	16.25	A
ATOM	1353	C	ILE	285	28.427	87.958	13.618	1.00	18.61	A
ATOM	1354	O	ILE	285	27.631	87.083	13.985	1.00	20.11	A
ATOM	1355	N	LEU	286	29.295	88.521	14.465	1.00	17.38	A
ATOM	1356	H	LEU	286	29.905	89.212	14.134	1.00	0.00	A
ATOM	1357	CA	LEU	286	29.348	88.131	15.884	1.00	17.79	A
ATOM	1358	CB	LEU	286	30.798	88.163	16.409	1.00	20.85	A
ATOM	1359	CG	LEU	286	31.846	87.099	16.069	1.00	23.26	A
ATOM	1360	CD1	LEU	286	32.975	87.139	17.093	1.00	26.78	A
ATOM	1361	CD2	LEU	286	31.217	85.739	16.067	1.00	25.33	A
ATOM	1362	C	LEU	286	28.501	89.056	16.754	1.00	18.17	A
ATOM	1363	O	LEU	286	28.515	88.951	17.983	1.00	20.22	A
ATOM	1364	N	GLY	287	27.788	89.969	16.099	1.00	22.67	A
ATOM	1365	H	GLY	287	27.840	89.999	15.120	1.00	0.00	A
ATOM	1366	CA	GLY	287	26.941	90.925	16.789	1.00	20.22	A
ATOM	1367	C	GLY	287	26.080	90.382	17.913	1.00	16.26	A
ATOM	1368	O	GLY	287	26.381	90.585	19.089	1.00	23.96	A
ATOM	1369	N	HIS	288	25.000	89.693	17.572	1.00	22.56	A
ATOM	1370	H	HIS	288	24.798	89.534	16.627	1.00	0.00	A
ATOM	1371	CA	HIS	288	24.109	89.168	18.608	1.00	20.44	A
ATOM	1372	CB	HIS	288	22.990	88.312	17.970	1.00	19.88	A
ATOM	1373	CG	HIS	288	21.974	87.804	18.950	1.00	23.39	A
ATOM	1374	CD2	HIS	288	21.917	86.650	19.654	1.00	17.27	A
ATOM	1375	ND1	HIS	288	20.917	88.571	19.385	1.00	15.20	A
ATOM	1376	HD1	HIS	288	20.679	89.455	19.045	1.00	0.00	A
ATOM	1377	CE1	HIS	288	20.242	87.909	20.310	1.00	15.13	A
ATOM	1378	NE2	HIS	288	20.832	86.739	20.494	1.00	13.24	A
ATOM	1379	HE2	HIS	288	20.535	86.056	21.118	1.00	0.00	A
ATOM	1380	C	HIS	288	24.850	88.371	19.715	1.00	17.46	A
ATOM	1381	O	HIS	288	24.579	88.541	20.902	1.00	17.25	A
ATOM	1382	N	TYR	289	25.798	87.525	19.334	1.00	18.14	A
ATOM	1383	H	TYR	289	26.023	87.431	18.384	1.00	0.00	A
ATOM	1384	CA	TYR	289	26.505	86.737	20.330	1.00	16.63	A
ATOM	1385	CB	TYR	289	27.405	85.709	19.647	1.00	25.01	A
ATOM	1386	CG	TYR	289	26.727	84.387	19.312	1.00	26.14	A
ATOM	1387	CD1	TYR	289	25.631	84.330	18.449	1.00	26.68	A
ATOM	1388	CE1	TYR	289	25.073	83.092	18.064	1.00	29.84	A
ATOM	1389	CD2	TYR	289	27.245	83.176	19.792	1.00	29.68	A
ATOM	1390	CE2	TYR	289	26.697	81.941	19.415	1.00	19.88	A
ATOM	1391	CZ	TYR	289	25.624	81.904	18.551	1.00	24.45	A
ATOM	1392	OH	TYR	289	25.129	80.680	18.154	1.00	29.76	A
ATOM	1393	HH	TYR	289	24.390	80.813	17.553	1.00	0.00	A
ATOM	1394	C	TYR	289	27.323	87.613	21.277	1.00	20.22	A
ATOM	1395	O	TYR	289	27.369	87.356	22.481	1.00	19.02	A

ATOM	1396	N	ASN	290	27.956	88.655	20.750	1.00	18.81	A
ATOM	1397	H	ASN	290	27.904	88.835	19.789	1.00	0.00	A
ATOM	1398	CA	ASN	290	28.739	89.532	21.621	1.00	15.76	A
ATOM	1399	CB	ASN	290	29.625	90.469	20.804	1.00	19.19	A
ATOM	1400	CG	ASN	290	30.840	89.780	20.231	1.00	22.46	A
ATOM	1401	OD1	ASN	290	31.270	88.736	20.715	1.00	23.52	A
ATOM	1402	ND2	ASN	290	31.400	90.370	19.186	1.00	25.92	A
ATOM	1403	HD21	ASN	290	31.020	91.202	18.832	1.00	0.00	A
ATOM	1404	HD22	ASN	290	32.188	89.942	18.796	1.00	0.00	A
ATOM	1405	C	ASN	290	27.822	90.378	22.493	1.00	15.64	A
ATOM	1406	O	ASN	290	28.108	90.600	23.672	1.00	23.61	A
ATOM	1407	N	ARG	291	26.723	90.865	21.924	1.00	15.28	A
ATOM	1408	H	ARG	291	26.524	90.672	20.984	1.00	0.00	A
ATOM	1409	CA	ARG	291	25.812	91.687	22.713	1.00	14.06	A
ATOM	1410	CB	ARG	291	24.679	92.252	21.845	1.00	16.24	A
ATOM	1411	CG	ARG	291	25.183	93.144	20.702	1.00	24.29	A
ATOM	1412	CD	ARG	291	24.091	94.025	20.084	1.00	29.20	A
ATOM	1413	NE	ARG	291	23.283	93.333	19.077	1.00	19.59	A
ATOM	1414	HE	ARG	291	22.365	93.092	19.317	1.00	0.00	A
ATOM	1415	CZ	ARG	291	23.709	93.013	17.859	1.00	34.23	A
ATOM	1416	NH1	ARG	291	24.948	93.323	17.484	1.00	34.45	A
ATOM	1417	HH11	ARG	291	25.559	93.796	18.117	1.00	0.00	A
ATOM	1418	HH12	ARG	291	25.268	93.078	16.568	1.00	0.00	A
ATOM	1419	NH2	ARG	291	22.898	92.381	17.014	1.00	30.49	A
ATOM	1420	HH21	ARG	291	21.967	92.149	17.292	1.00	0.00	A
ATOM	1421	HH22	ARG	291	23.222	92.139	16.099	1.00	0.00	A
ATOM	1422	C	ARG	291	25.268	90.835	23.845	1.00	12.25	A
ATOM	1423	O	ARG	291	25.073	91.317	24.963	1.00	17.10	A
ATOM	1424	N	GLY	292	25.073	89.551	23.576	1.00	13.55	A
ATOM	1425	H	GLY	292	25.286	89.193	22.690	1.00	0.00	A
ATOM	1426	CA	GLY	292	24.534	88.675	24.616	1.00	11.54	A
ATOM	1427	C	GLY	292	25.542	88.057	25.562	1.00	22.48	A
ATOM	1428	O	GLY	292	25.169	87.246	26.411	1.00	30.06	A
ATOM	1429	N	ASN	293	26.813	88.425	25.422	1.00	25.61	A
ATOM	1430	H	ASN	293	27.049	89.065	24.719	1.00	0.00	A
ATOM	1431	CA	ASN	293	27.867	87.897	26.281	1.00	29.06	A
ATOM	1432	CB	ASN	293	27.567	88.238	27.750	1.00	33.48	A
ATOM	1433	CG	ASN	293	27.687	89.741	28.058	1.00	41.34	A
ATOM	1434	OD1	ASN	293	27.506	90.595	27.185	1.00	41.61	A
ATOM	1435	ND2	ASN	293	27.988	90.060	29.319	1.00	40.94	A
ATOM	1436	HD21	ASN	293	28.120	89.353	29.985	1.00	0.00	A
ATOM	1437	HD22	ASN	293	28.069	91.011	29.537	1.00	0.00	A
ATOM	1438	C	ASN	293	28.042	86.369	26.116	1.00	31.86	A
ATOM	1439	O	ASN	293	28.265	85.652	27.093	1.00	25.49	A
ATOM	1440	N	LEU	294	27.952	85.884	24.877	1.00	35.13	A
ATOM	1441	H	LEU	294	27.777	86.501	24.138	1.00	0.00	A
ATOM	1442	CA	LEU	294	28.102	84.456	24.588	1.00	33.84	A
ATOM	1443	CB	LEU	294	26.918	83.942	23.747	1.00	34.45	A
ATOM	1444	CG	LEU	294	25.482	84.323	24.145	1.00	35.78	A
ATOM	1445	CD1	LEU	294	24.601	84.404	22.911	1.00	35.34	A
ATOM	1446	CD2	LEU	294	24.923	83.299	25.121	1.00	34.64	A
ATOM	1447	C	LEU	294	29.415	84.154	23.852	1.00	37.21	A
ATOM	1448	O	LEU	294	29.957	85.002	23.137	1.00	32.23	A
ATOM	1449	N	SER	295	29.930	82.943	24.056	1.00	38.58	A
ATOM	1450	H	SER	295	29.465	82.328	24.659	1.00	0.00	A
ATOM	1451	CA	SER	295	31.163	82.499	23.409	1.00	38.66	A
ATOM	1452	CB	SER	295	31.590	81.113	23.930	1.00	40.11	A
ATOM	1453	OG	SER	295	31.942	81.141	25.306	1.00	45.34	A
ATOM	1454	HG	SER	295	31.187	81.434	25.822	1.00	0.00	A
ATOM	1455	C	SER	295	30.881	82.404	21.914	1.00	33.43	A
ATOM	1456	O	SER	295	29.780	82.064	21.499	1.00	25.91	A
ATOM	1457	N	THR	296	31.881	82.703	21.107	1.00	34.10	A
ATOM	1458	H	THR	296	32.745	82.966	21.488	1.00	0.00	A
ATOM	1459	CA	THR	296	31.722	82.649	19.670	1.00	32.52	A
ATOM	1460	CB	THR	296	31.966	84.030	19.052	1.00	30.78	A
ATOM	1461	OG1	THR	296	33.072	84.647	19.717	1.00	36.83	A
ATOM	1462	HG1	THR	296	33.856	84.103	19.610	1.00	0.00	A
ATOM	1463	CG2	THR	296	30.740	84.916	19.220	1.00	29.89	A
ATOM	1464	C	THR	296	32.759	81.673	19.155	1.00	31.85	A
ATOM	1465	O	THR	296	32.898	81.483	17.952	1.00	31.90	A
ATOM	1466	N	GLU	297	33.482	81.059	20.089	1.00	33.84	A
ATOM	1467	H	GLU	297	33.304	81.261	21.032	1.00	0.00	A
ATOM	1468	CA	GLU	297	34.531	80.096	19.763	1.00	39.29	A

ATOM	1469	CB	GLU	297	35.065	79.416	21.036	1.00	45.48	A
ATOM	1470	CG	GLU	297	34.108	79.377	22.233	1.00	56.35	A
ATOM	1471	CD	GLU	297	32.848	78.554	21.977	1.00	58.88	A
ATOM	1472	OE1	GLU	297	32.842	77.338	22.267	1.00	60.54	A
ATOM	1473	OE2	GLU	297	31.855	79.130	21.489	1.00	62.33	A
ATOM	1474	C	GLU	297	34.086	79.024	18.772	1.00	35.45	A
ATOM	1475	O	GLU	297	34.729	78.809	17.748	1.00	34.80	A
ATOM	1476	N	LYS	298	32.982	78.356	19.074	1.00	34.37	A
ATOM	1477	H	LYS	298	32.498	78.581	19.895	1.00	0.00	A
ATOM	1478	CA	LYS	298	32.466	77.300	18.213	1.00	35.58	A
ATOM	1479	CB	LYS	298	31.520	76.414	19.007	1.00	31.26	A
ATOM	1480	CG	LYS	298	32.038	75.026	19.221	1.00	41.82	A
ATOM	1481	CD	LYS	298	30.941	74.125	19.729	1.00	42.14	A
ATOM	1482	CE	LYS	298	31.135	73.832	21.200	1.00	46.89	A
ATOM	1483	NZ	LYS	298	32.466	74.301	21.688	1.00	50.64	A
ATOM	1484	HZ1	LYS	298	32.544	75.328	21.550	1.00	0.00	A
ATOM	1485	HZ2	LYS	298	33.219	73.820	21.158	1.00	0.00	A
ATOM	1486	HZ3	LYS	298	32.559	74.079	22.701	1.00	0.00	A
ATOM	1487	C	LYS	298	31.743	77.850	16.992	1.00	31.74	A
ATOM	1488	O	LYS	298	31.765	77.236	15.922	1.00	32.24	A
ATOM	1489	N	PHE	299	31.101	79.005	17.170	1.00	29.34	A
ATOM	1490	H	PHE	299	31.131	79.425	18.053	1.00	0.00	A
ATOM	1491	CA	PHE	299	30.353	79.673	16.102	1.00	28.31	A
ATOM	1492	CB	PHE	299	29.612	80.883	16.703	1.00	27.71	A
ATOM	1493	CG	PHE	299	29.131	81.904	15.699	1.00	19.45	A
ATOM	1494	CD1	PHE	299	28.503	81.526	14.516	1.00	15.16	A
ATOM	1495	CD2	PHE	299	29.287	83.261	15.964	1.00	16.16	A
ATOM	1496	CE1	PHE	299	28.046	82.496	13.616	1.00	15.54	A
ATOM	1497	CE2	PHE	299	28.832	84.227	15.075	1.00	9.30	A
ATOM	1498	CZ	PHE	299	28.215	83.851	13.903	1.00	7.56	A
ATOM	1499	C	PHE	299	31.296	80.076	14.966	1.00	27.62	A
ATOM	1500	O	PHE	299	30.999	79.828	13.803	1.00	23.92	A
ATOM	1501	N	VAL	300	32.440	80.667	15.300	1.00	32.50	A
ATOM	1502	H	VAL	300	32.635	80.834	16.246	1.00	0.00	A
ATOM	1503	CA	VAL	300	33.419	81.074	14.280	1.00	40.70	A
ATOM	1504	CB	VAL	300	34.545	81.950	14.877	1.00	45.83	A
ATOM	1505	CG1	VAL	300	35.734	81.084	15.280	1.00	49.69	A
ATOM	1506	CG2	VAL	300	34.988	82.975	13.860	1.00	49.35	A
ATOM	1507	C	VAL	300	34.082	79.887	13.575	1.00	39.59	A
ATOM	1508	O	VAL	300	34.426	79.974	12.399	1.00	39.52	A
ATOM	1509	N	GLU	301	34.274	78.791	14.302	1.00	38.31	A
ATOM	1510	H	GLU	301	34.001	78.787	15.244	1.00	0.00	A
ATOM	1511	CA	GLU	301	34.879	77.597	13.736	1.00	39.63	A
ATOM	1512	CB	GLU	301	35.240	76.607	14.849	1.00	49.28	A
ATOM	1513	CG	GLU	301	36.060	75.406	14.388	1.00	51.49	A
ATOM	1514	CD	GLU	301	35.928	74.221	15.328	1.00	57.74	A
ATOM	1515	OE1	GLU	301	34.879	73.542	15.283	1.00	60.72	A
ATOM	1516	OE2	GLU	301	36.867	73.968	16.114	1.00	58.47	A
ATOM	1517	C	GLU	301	33.933	76.932	12.742	1.00	37.25	A
ATOM	1518	O	GLU	301	34.360	76.469	11.695	1.00	34.80	A
ATOM	1519	N	GLU	302	32.647	76.880	13.061	1.00	29.99	A
ATOM	1520	H	GLU	302	32.332	77.260	13.909	1.00	0.00	A
ATOM	1521	CA	GLU	302	31.713	76.254	12.144	1.00	29.62	A
ATOM	1522	CB	GLU	302	30.345	76.072	12.800	1.00	29.29	A
ATOM	1523	CG	GLU	302	29.188	76.118	11.813	1.00	30.24	A
ATOM	1524	CD	GLU	302	27.839	76.218	12.489	1.00	26.05	A
ATOM	1525	OE1	GLU	302	27.674	75.643	13.581	1.00	24.89	A
ATOM	1526	OE2	GLU	302	26.940	76.870	11.925	1.00	30.75	A
ATOM	1527	C	GLU	302	31.574	77.093	10.874	1.00	32.99	A
ATOM	1528	O	GLU	302	31.445	76.549	9.775	1.00	30.91	A
ATOM	1529	N	ILE	303	31.615	78.416	11.014	1.00	31.38	A
ATOM	1530	H	ILE	303	31.732	78.810	11.904	1.00	0.00	A
ATOM	1531	CA	ILE	303	31.486	79.283	9.842	1.00	31.29	A
ATOM	1532	CB	ILE	303	31.187	80.752	10.241	1.00	28.58	A
ATOM	1533	CG2	ILE	303	30.822	81.554	9.009	1.00	23.48	A
ATOM	1534	CG1	ILE	303	30.043	80.800	11.264	1.00	26.97	A
ATOM	1535	CD1	ILE	303	28.805	80.026	10.852	1.00	24.95	A
ATOM	1536	C	ILE	303	32.773	79.228	9.029	1.00	33.05	A
ATOM	1537	O	ILE	303	32.744	79.181	7.796	1.00	35.02	A
ATOM	1538	N	LYS	304	33.903	79.248	9.724	1.00	30.79	A
ATOM	1539	H	LYS	304	33.869	79.332	10.698	1.00	0.00	A
ATOM	1540	CA	LYS	304	35.190	79.150	9.060	1.00	30.72	A
ATOM	1541	CB	LYS	304	36.298	78.979	10.118	1.00	33.59	A

```
ATOM   1542  CG  LYS   304      37.724  79.320   9.642  1.00 41.97      A
ATOM   1543  CD  LYS   304      38.511  80.155  10.667  1.00 41.17      A
ATOM   1544  CE  LYS   304      39.416  81.173   9.976  1.00 42.05      A
ATOM   1545  NZ  LYS   304      40.815  80.691   9.824  1.00 41.08      A
ATOM   1546  HZ1 LYS   304      40.823  79.820   9.256  1.00  0.00      A
ATOM   1547  HZ2 LYS   304      41.217  80.495  10.764  1.00  0.00      A
ATOM   1548  HZ3 LYS   304      41.384  81.421   9.350  1.00  0.00      A
ATOM   1549  C   LYS   304      35.100  77.904   8.161  1.00 25.59      A
ATOM   1550  O   LYS   304      35.395  77.951   6.969  1.00 33.47      A
ATOM   1551  N   SER   305      34.661  76.800   8.767  1.00 26.69      A
ATOM   1552  H   SER   305      34.433  76.870   9.716  1.00  0.00      A
ATOM   1553  CA  SER   305      34.498  75.489   8.125  1.00 22.76      A
ATOM   1554  CB  SER   305      33.932  74.498   9.144  1.00 27.40      A
ATOM   1555  OG  SER   305      32.539  74.298   8.939  1.00 24.13      A
ATOM   1556  HG  SER   305      32.075  75.133   9.030  1.00  0.00      A
ATOM   1557  C   SER   305      33.635  75.403   6.860  1.00 24.66      A
ATOM   1558  O   SER   305      33.536  74.340   6.239  1.00 27.99      A
ATOM   1559  N   ILE   306      32.983  76.490   6.482  1.00 25.24      A
ATOM   1560  H   ILE   306      33.058  77.317   7.005  1.00  0.00      A
ATOM   1561  CA  ILE   306      32.154  76.453   5.294  1.00 20.72      A
ATOM   1562  CB  ILE   306      30.828  77.211   5.513  1.00 17.86      A
ATOM   1563  CG2 ILE   306      30.078  77.326   4.209  1.00 20.63      A
ATOM   1564  CG1 ILE   306      29.952  76.448   6.510  1.00 20.49      A
ATOM   1565  CD1 ILE   306      29.382  77.307   7.603  1.00 19.14      A
ATOM   1566  C   ILE   306      32.908  77.098   4.156  1.00 16.50      A
ATOM   1567  O   ILE   306      32.689  76.783   2.994  1.00 19.41      A
ATOM   1568  N   ALA   307      33.833  77.979   4.499  1.00 22.89      A
ATOM   1569  H   ALA   307      34.019  78.150   5.446  1.00  0.00      A
ATOM   1570  CA  ALA   307      34.576  78.686   3.480  1.00 24.83      A
ATOM   1571  CB  ALA   307      35.383  79.794   4.123  1.00 30.01      A
ATOM   1572  C   ALA   307      35.476  77.766   2.665  1.00 23.99      A
ATOM   1573  O   ALA   307      36.047  76.812   3.187  1.00 21.83      A
ATOM   1574  N   SER   308      35.568  78.035   1.368  1.00 23.95      A
ATOM   1575  H   SER   308      35.037  78.765   0.987  1.00  0.00      A
ATOM   1576  CA  SER   308      36.445  77.252   0.511  1.00 29.22      A
ATOM   1577  CB  SER   308      36.343  77.740  -0.937  1.00 21.79      A
ATOM   1578  OG  SER   308      35.241  77.145  -1.606  1.00 28.41      A
ATOM   1579  HG  SER   308      34.430  77.376  -1.149  1.00  0.00      A
ATOM   1580  C   SER   308      37.870  77.489   1.035  1.00 34.88      A
ATOM   1581  O   SER   308      38.119  78.483   1.724  1.00 32.75      A
ATOM   1582  N   GLU   309      38.795  76.581   0.722  1.00 40.30      A
ATOM   1583  H   GLU   309      38.537  75.801   0.188  1.00  0.00      A
ATOM   1584  CA  GLU   309      40.191  76.729   1.160  1.00 42.81      A
ATOM   1585  CB  GLU   309      40.931  75.385   1.086  1.00 46.85      A
ATOM   1586  CG  GLU   309      40.454  74.318   2.062  1.00 53.06      A
ATOM   1587  CD  GLU   309      41.310  74.231   3.318  1.00 57.34      A
ATOM   1588  OE1 GLU   309      42.553  74.307   3.215  1.00 58.52      A
ATOM   1589  OE2 GLU   309      40.734  74.085   4.416  1.00 61.40      A
ATOM   1590  C   GLU   309      40.861  77.715   0.205  1.00 43.24      A
ATOM   1591  O   GLU   309      40.550  77.718  -0.987  1.00 44.53      A
ATOM   1592  N   PRO   310      41.762  78.581   0.706  1.00 40.58      A
ATOM   1593  CD  PRO   310      42.414  79.532  -0.216  1.00 41.03      A
ATOM   1594  CA  PRO   310      42.250  78.757   2.080  1.00 41.16      A
ATOM   1595  CB  PRO   310      43.538  79.545   1.899  1.00 43.29      A
ATOM   1596  CG  PRO   310      43.269  80.379   0.695  1.00 42.72      A
ATOM   1597  C   PRO   310      41.242  79.519   2.942  1.00 41.57      A
ATOM   1598  O   PRO   310      40.758  80.582   2.553  1.00 35.45      A
ATOM   1599  N   THR   311      40.953  78.976   4.118  1.00 40.54      A
ATOM   1600  H   THR   311      41.400  78.144   4.378  1.00  0.00      A
ATOM   1601  CA  THR   311      39.991  79.574   5.033  1.00 40.87      A
ATOM   1602  CB  THR   311      39.893  78.738   6.311  1.00 39.66      A
ATOM   1603  OG1 THR   311      39.391  79.549   7.377  1.00 46.71      A
ATOM   1604  HG1 THR   311      38.520  79.880   7.146  1.00  0.00      A
ATOM   1605  CG2 THR   311      41.258  78.200   6.690  1.00 43.68      A
ATOM   1606  C   THR   311      40.246  81.037   5.413  1.00 44.47      A
ATOM   1607  O   THR   311      39.299  81.802   5.620  1.00 45.91      A
ATOM   1608  N   GLU   312      41.514  81.432   5.510  1.00 45.09      A
ATOM   1609  H   GLU   312      42.234  80.792   5.337  1.00  0.00      A
ATOM   1610  CA  GLU   312      41.839  82.809   5.871  1.00 42.55      A
ATOM   1611  CB  GLU   312      43.327  82.954   6.228  1.00 42.74      A
ATOM   1612  CG  GLU   312      44.235  81.829   5.726  1.00 43.79      A
ATOM   1613  CD  GLU   312      44.520  80.800   6.799  1.00 41.47      A
ATOM   1614  OE1 GLU   312      45.706  80.520   7.057  1.00 42.55      A
```

ATOM	1615	OE2	GLU	312	43.559	80.274	7.394	1.00	47.20	A
ATOM	1616	C	GLU	312	41.502	83.747	4.724	1.00	41.45	A
ATOM	1617	O	GLU	312	41.404	84.963	4.901	1.00	41.26	A
ATOM	1618	N	LYS	313	41.317	83.181	3.542	1.00	37.88	A
ATOM	1619	H	LYS	313	41.394	82.207	3.451	1.00	0.00	A
ATOM	1620	CA	LYS	313	40.997	83.993	2.380	1.00	36.21	A
ATOM	1621	CB	LYS	313	41.564	83.358	1.116	1.00	33.23	A
ATOM	1622	CG	LYS	313	41.563	84.300	-0.079	1.00	34.65	A
ATOM	1623	CD	LYS	313	41.058	83.617	-1.335	1.00	27.45	A
ATOM	1624	CE	LYS	313	39.861	84.348	-1.905	1.00	29.91	A
ATOM	1625	NZ	LYS	313	39.913	84.435	-3.387	1.00	32.98	A
ATOM	1626	HZ1	LYS	313	39.928	83.476	-3.790	1.00	0.00	A
ATOM	1627	HZ2	LYS	313	40.770	84.946	-3.674	1.00	0.00	A
ATOM	1628	HZ3	LYS	313	39.073	84.941	-3.733	1.00	0.00	A
ATOM	1629	C	LYS	313	39.515	84.249	2.159	1.00	37.37	A
ATOM	1630	O	LYS	313	39.132	85.357	1.789	1.00	40.91	A
ATOM	1631	N	HIS	314	38.683	83.234	2.385	1.00	32.67	A
ATOM	1632	H	HIS	314	39.036	82.382	2.718	1.00	0.00	A
ATOM	1633	CA	HIS	314	37.250	83.372	2.143	1.00	34.37	A
ATOM	1634	CB	HIS	314	36.725	82.171	1.343	1.00	33.80	A
ATOM	1635	CG	HIS	314	37.658	81.682	0.280	1.00	29.70	A
ATOM	1636	CD2	HIS	314	38.910	81.168	0.360	1.00	31.43	A
ATOM	1637	ND1	HIS	314	37.307	81.631	-1.051	1.00	29.34	A
ATOM	1638	HD1	HIS	314	36.455	81.936	-1.435	1.00	0.00	A
ATOM	1639	CE1	HIS	314	38.295	81.109	-1.747	1.00	29.33	A
ATOM	1640	NE2	HIS	314	39.283	80.818	-0.914	1.00	29.14	A
ATOM	1641	HE2	HIS	314	40.137	80.421	-1.175	1.00	0.00	A
ATOM	1642	C	HIS	314	36.368	83.552	3.372	1.00	35.91	A
ATOM	1643	O	HIS	314	35.184	83.860	3.239	1.00	41.62	A
ATOM	1644	N	PHE	315	36.920	83.340	4.559	1.00	36.72	A
ATOM	1645	H	PHE	315	37.858	83.065	4.622	1.00	0.00	A
ATOM	1646	CA	PHE	315	36.132	83.512	5.770	1.00	37.19	A
ATOM	1647	CB	PHE	315	36.552	82.493	6.834	1.00	34.33	A
ATOM	1648	CG	PHE	315	36.038	82.804	8.214	1.00	26.72	A
ATOM	1649	CD1	PHE	315	34.684	82.672	8.519	1.00	30.96	A
ATOM	1650	CD2	PHE	315	36.911	83.225	9.213	1.00	25.93	A
ATOM	1651	CE1	PHE	315	34.209	82.955	9.800	1.00	23.91	A
ATOM	1652	CE2	PHE	315	36.451	83.510	10.494	1.00	28.16	A
ATOM	1653	CZ	PHE	315	35.094	83.375	10.788	1.00	29.32	A
ATOM	1654	C	PHE	315	36.326	84.928	6.299	1.00	38.47	A
ATOM	1655	O	PHE	315	37.449	85.428	6.344	1.00	41.30	A
ATOM	1656	N	PHE	316	35.219	85.561	6.685	1.00	36.02	A
ATOM	1657	H	PHE	316	34.364	85.091	6.602	1.00	0.00	A
ATOM	1658	CA	PHE	316	35.213	86.918	7.223	1.00	32.16	A
ATOM	1659	CB	PHE	316	34.390	87.856	6.334	1.00	31.62	A
ATOM	1660	CG	PHE	316	35.057	88.194	5.041	1.00	37.01	A
ATOM	1661	CD1	PHE	316	34.804	87.437	3.898	1.00	29.79	A
ATOM	1662	CD2	PHE	316	35.979	89.233	4.971	1.00	33.37	A
ATOM	1663	CE1	PHE	316	35.462	87.705	2.713	1.00	33.51	A
ATOM	1664	CE2	PHE	316	36.644	89.511	3.786	1.00	37.63	A
ATOM	1665	CZ	PHE	316	36.388	88.745	2.653	1.00	37.22	A
ATOM	1666	C	PHE	316	34.577	86.895	8.596	1.00	30.46	A
ATOM	1667	O	PHE	316	33.446	86.467	8.751	1.00	28.70	A
ATOM	1668	N	ASN	317	35.311	87.355	9.591	1.00	30.17	A
ATOM	1669	H	ASN	317	36.220	87.668	9.414	1.00	0.00	A
ATOM	1670	CA	ASN	317	34.795	87.405	10.939	1.00	31.72	A
ATOM	1671	CB	ASN	317	35.855	86.917	11.927	1.00	29.33	A
ATOM	1672	CG	ASN	317	35.485	87.205	13.376	1.00	34.11	A
ATOM	1673	OD1	ASN	317	34.771	88.163	13.667	1.00	38.43	A
ATOM	1674	ND2	ASN	317	35.983	86.375	14.289	1.00	32.35	A
ATOM	1675	HD21	ASN	317	36.553	85.627	14.018	1.00	0.00	A
ATOM	1676	HD22	ASN	317	35.752	86.550	15.226	1.00	0.00	A
ATOM	1677	C	ASN	317	34.442	88.861	11.197	1.00	33.41	A
ATOM	1678	O	ASN	317	35.325	89.686	11.440	1.00	35.10	A
ATOM	1679	N	VAL	318	33.152	89.175	11.128	1.00	34.27	A
ATOM	1680	H	VAL	318	32.498	88.478	10.922	1.00	0.00	A
ATOM	1681	CA	VAL	318	32.689	90.543	11.355	1.00	32.08	A
ATOM	1682	CB	VAL	318	31.629	90.958	10.301	1.00	36.04	A
ATOM	1683	CG1	VAL	318	31.316	92.441	10.426	1.00	35.17	A
ATOM	1684	CG2	VAL	318	32.147	90.660	8.905	1.00	37.95	A
ATOM	1685	C	VAL	318	32.123	90.743	12.762	1.00	25.89	A
ATOM	1686	O	VAL	318	31.293	89.978	13.238	1.00	27.33	A
ATOM	1687	N	SER	319	32.618	91.790	13.406	1.00	23.18	A

ATOM	1688	H	SER	319	33.278	92.338	12.932	1.00	0.00	A
ATOM	1689	CA	SER	319	32.261	92.198	14.757	1.00	22.35	A
ATOM	1690	CB	SER	319	32.972	93.523	15.071	1.00	21.96	A
ATOM	1691	OG	SER	319	33.554	93.517	16.360	1.00	35.71	A
ATOM	1692	HG	SER	319	34.201	92.809	16.416	1.00	0.00	A
ATOM	1693	C	SER	319	30.765	92.371	14.988	1.00	22.88	A
ATOM	1694	O	SER	319	30.212	91.854	15.959	1.00	20.95	A
ATOM	1695	N	ASP	320	30.128	93.157	14.125	1.00	25.15	A
ATOM	1696	H	ASP	320	30.632	93.579	13.399	1.00	0.00	A
ATOM	1697	CA	ASP	320	28.698	93.400	14.232	1.00	23.64	A
ATOM	1698	CB	ASP	320	28.383	94.447	15.334	1.00	30.33	A
ATOM	1699	CG	ASP	320	29.128	95.762	15.156	1.00	27.91	A
ATOM	1700	OD1	ASP	320	30.369	95.774	15.088	1.00	27.84	A
ATOM	1701	OD2	ASP	320	28.456	96.799	15.098	1.00	30.37	A
ATOM	1702	C	ASP	320	28.093	93.791	12.896	1.00	21.79	A
ATOM	1703	O	ASP	320	28.796	93.896	11.893	1.00	21.85	A
ATOM	1704	N	GLU	321	26.781	93.982	12.878	1.00	23.98	A
ATOM	1705	H	GLU	321	26.274	93.890	13.711	1.00	0.00	A
ATOM	1706	CA	GLU	321	26.077	94.326	11.652	1.00	25.27	A
ATOM	1707	CB	GLU	321	24.565	94.361	11.920	1.00	24.89	A
ATOM	1708	CG	GLU	321	23.954	92.980	12.285	1.00	16.77	A
ATOM	1709	CD	GLU	321	23.945	92.711	13.793	1.00	16.37	A
ATOM	1710	OE1	GLU	321	24.672	93.402	14.533	1.00	17.10	A
ATOM	1711	OE2	GLU	321	23.203	91.815	14.244	1.00	21.60	A
ATOM	1712	C	GLU	321	26.547	95.638	11.019	1.00	30.46	A
ATOM	1713	O	GLU	321	26.682	95.733	9.795	1.00	26.52	A
ATOM	1714	N	LEU	322	26.804	96.649	11.847	1.00	30.02	A
ATOM	1715	H	LEU	322	26.680	96.524	12.809	1.00	0.00	A
ATOM	1716	CA	LEU	322	27.266	97.937	11.338	1.00	33.52	A
ATOM	1717	CB	LEU	322	27.371	98.959	12.480	1.00	24.65	A
ATOM	1718	CG	LEU	322	26.103	99.774	12.671	1.00	21.95	A
ATOM	1719	CD1	LEU	322	26.344	100.939	13.616	1.00	25.01	A
ATOM	1720	CD2	LEU	322	25.653	100.267	11.323	1.00	29.24	A
ATOM	1721	C	LEU	322	28.620	97.824	10.632	1.00	34.43	A
ATOM	1722	O	LEU	322	28.860	98.497	9.630	1.00	38.95	A
ATOM	1723	N	ALA	323	29.492	96.962	11.142	1.00	35.14	A
ATOM	1724	H	ALA	323	29.236	96.426	11.923	1.00	0.00	A
ATOM	1725	CA	ALA	323	30.826	96.790	10.569	1.00	35.03	A
ATOM	1726	CB	ALA	323	31.768	96.217	11.625	1.00	35.40	A
ATOM	1727	C	ALA	323	30.880	95.925	9.311	1.00	35.38	A
ATOM	1728	O	ALA	323	31.967	95.531	8.878	1.00	34.45	A
ATOM	1729	N	LEU	324	29.718	95.632	8.730	1.00	33.27	A
ATOM	1730	H	LEU	324	28.891	95.981	9.121	1.00	0.00	A
ATOM	1731	CA	LEU	324	29.638	94.805	7.525	1.00	30.65	A
ATOM	1732	CB	LEU	324	28.199	94.313	7.308	1.00	28.08	A
ATOM	1733	CG	LEU	324	27.672	92.979	7.874	1.00	27.13	A
ATOM	1734	CD1	LEU	324	26.168	92.949	7.666	1.00	24.21	A
ATOM	1735	CD2	LEU	324	28.304	91.773	7.178	1.00	24.75	A
ATOM	1736	C	LEU	324	30.086	95.604	6.296	1.00	37.04	A
ATOM	1737	O	LEU	324	30.858	95.116	5.471	1.00	31.90	A
ATOM	1738	N	VAL	325	29.601	96.841	6.193	1.00	40.73	A
ATOM	1739	H	VAL	325	29.010	97.174	6.898	1.00	0.00	A
ATOM	1740	CA	VAL	325	29.923	97.711	5.069	1.00	43.41	A
ATOM	1741	CB	VAL	325	29.063	98.996	5.093	1.00	46.34	A
ATOM	1742	CG1	VAL	325	27.959	98.896	4.052	1.00	47.62	A
ATOM	1743	CG2	VAL	325	28.470	99.209	6.474	1.00	51.12	A
ATOM	1744	C	VAL	325	31.395	98.107	4.985	1.00	46.86	A
ATOM	1745	O	VAL	325	31.759	99.028	4.248	1.00	48.27	A
ATOM	1746	N	THR	326	32.241	97.409	5.736	1.00	45.92	A
ATOM	1747	H	THR	326	31.892	96.697	6.310	1.00	0.00	A
ATOM	1748	CA	THR	326	33.672	97.677	5.729	1.00	48.06	A
ATOM	1749	CB	THR	326	34.180	98.101	7.125	1.00	49.74	A
ATOM	1750	OG1	THR	326	34.656	96.949	7.830	1.00	53.08	A
ATOM	1751	HG1	THR	326	33.943	96.315	7.928	1.00	0.00	A
ATOM	1752	CG2	THR	326	33.063	98.756	7.926	1.00	52.68	A
ATOM	1753	C	THR	326	34.411	96.415	5.313	1.00	47.66	A
ATOM	1754	O	THR	326	35.615	96.290	5.523	1.00	45.71	A
ATOM	1755	N	ILE	327	33.675	95.479	4.725	1.00	50.08	A
ATOM	1756	H	ILE	327	32.720	95.648	4.586	1.00	0.00	A
ATOM	1757	CA	ILE	327	34.239	94.211	4.278	1.00	49.17	A
ATOM	1758	CB	ILE	327	33.653	93.029	5.118	1.00	46.23	A
ATOM	1759	CG2	ILE	327	32.917	92.026	4.237	1.00	47.06	A
ATOM	1760	CG1	ILE	327	34.779	92.352	5.895	1.00	47.16	A

```
ATOM   1761  CD1 ILE   327      34.325  91.201   6.768  1.00 44.14      A
ATOM   1762  C   ILE   327      33.936  94.026   2.793  1.00 50.56      A
ATOM   1763  O   ILE   327      34.327  93.026   2.179  1.00 50.93      A
ATOM   1764  N   VAL   328      33.261  95.020   2.220  1.00 49.92      A
ATOM   1765  H   VAL   328      33.014  95.796   2.765  1.00  0.00      A
ATOM   1766  CA  VAL   328      32.878  94.998   0.812  1.00 53.12      A
ATOM   1767  CB  VAL   328      31.947  96.172   0.479  1.00 51.75      A
ATOM   1768  CG1 VAL   328      30.573  95.931   1.085  1.00 53.91      A
ATOM   1769  CG2 VAL   328      32.552  97.465   1.000  1.00 52.78      A
ATOM   1770  C   VAL   328      34.045  95.043  -0.173  1.00 54.61      A
ATOM   1771  O   VAL   328      33.974  94.456  -1.252  1.00 53.08      A
ATOM   1772  N   LYS   329      35.114  95.745   0.190  1.00 56.00      A
ATOM   1773  H   LYS   329      35.130  96.192   1.061  1.00  0.00      A
ATOM   1774  CA  LYS   329      36.262  95.855  -0.699  1.00 54.78      A
ATOM   1775  CB  LYS   329      37.185  96.987  -0.239  1.00 59.48      A
ATOM   1776  CG  LYS   329      37.135  98.218  -1.130  1.00 62.07      A
ATOM   1777  CD  LYS   329      35.950  99.103  -0.777  1.00 64.89      A
ATOM   1778  CE  LYS   329      34.651  98.580  -1.372  1.00 68.36      A
ATOM   1779  NZ  LYS   329      34.865  97.635  -2.509  1.00 71.98      A
ATOM   1780  HZ1 LYS   329      35.410  96.815  -2.184  1.00  0.00      A
ATOM   1781  HZ2 LYS   329      35.385  98.117  -3.268  1.00  0.00      A
ATOM   1782  HZ3 LYS   329      33.943  97.314  -2.871  1.00  0.00      A
ATOM   1783  C   LYS   329      37.053  94.565  -0.841  1.00 51.87      A
ATOM   1784  O   LYS   329      37.406  94.173  -1.954  1.00 52.46      A
ATOM   1785  N   ALA   330      37.320  93.902   0.280  1.00 47.32      A
ATOM   1786  H   ALA   330      36.995  94.257   1.134  1.00  0.00      A
ATOM   1787  CA  ALA   330      38.085  92.663   0.264  1.00 46.18      A
ATOM   1788  CB  ALA   330      38.581  92.348   1.659  1.00 42.75      A
ATOM   1789  C   ALA   330      37.299  91.476  -0.287  1.00 47.64      A
ATOM   1790  O   ALA   330      37.877  90.567  -0.876  1.00 47.07      A
ATOM   1791  N   LEU   331      35.984  91.484  -0.089  1.00 49.91      A
ATOM   1792  H   LEU   331      35.578  92.237   0.390  1.00  0.00      A
ATOM   1793  CA  LEU   331      35.125  90.398  -0.568  1.00 46.71      A
ATOM   1794  CB  LEU   331      33.767  90.437   0.145  1.00 41.67      A
ATOM   1795  CG  LEU   331      32.981  89.151   0.428  1.00 37.35      A
ATOM   1796  CD1 LEU   331      31.508  89.445   0.260  1.00 38.69      A
ATOM   1797  CD2 LEU   331      33.395  88.028  -0.493  1.00 32.33      A
ATOM   1798  C   LEU   331      34.906  90.563  -2.060  1.00 46.57      A
ATOM   1799  O   LEU   331      34.938  89.595  -2.817  1.00 44.39      A
ATOM   1800  N   GLY   332      34.683  91.808  -2.462  1.00 47.56      A
ATOM   1801  H   GLY   332      34.682  92.530  -1.800  1.00  0.00      A
ATOM   1802  CA  GLY   332      34.443  92.127  -3.853  1.00 48.35      A
ATOM   1803  C   GLY   332      35.651  91.998  -4.753  1.00 49.41      A
ATOM   1804  O   GLY   332      35.512  92.028  -5.974  1.00 54.37      A
ATOM   1805  N   GLU   333      36.840  91.870  -4.177  1.00 48.21      A
ATOM   1806  H   GLU   333      36.918  91.872  -3.200  1.00  0.00      A
ATOM   1807  CA  GLU   333      38.023  91.727  -5.008  1.00 44.83      A
ATOM   1808  CB  GLU   333      39.113  92.733  -4.593  1.00 44.79      A
ATOM   1809  CG  GLU   333      40.169  92.276  -3.598  1.00 44.17      A
ATOM   1810  CD  GLU   333      40.917  93.463  -2.986  1.00 43.91      A
ATOM   1811  OE1 GLU   333      41.368  93.370  -1.825  1.00 47.51      A
ATOM   1812  OE2 GLU   333      41.048  94.499  -3.668  1.00 36.94      A
ATOM   1813  C   GLU   333      38.506  90.289  -4.953  1.00 42.92      A
ATOM   1814  O   GLU   333      38.945  89.735  -5.965  1.00 41.97      A
ATOM   1815  N   ARG   334      38.387  89.669  -3.784  1.00 35.56      A
ATOM   1816  H   ARG   334      38.029  90.155  -3.013  1.00  0.00      A
ATOM   1817  CA  ARG   334      38.789  88.274  -3.638  1.00 41.85      A
ATOM   1818  CB  ARG   334      38.733  87.861  -2.171  1.00 39.37      A
ATOM   1819  CG  ARG   334      39.742  88.555  -1.305  1.00 38.56      A
ATOM   1820  CD  ARG   334      39.589  88.107   0.118  1.00 37.12      A
ATOM   1821  NE  ARG   334      40.288  88.994   1.029  1.00 29.46      A
ATOM   1822  HE  ARG   334      40.713  89.795   0.661  1.00  0.00      A
ATOM   1823  CZ  ARG   334      40.367  88.791   2.338  1.00 34.98      A
ATOM   1824  NH1 ARG   334      39.786  87.737   2.880  1.00 31.07      A
ATOM   1825 HH11 ARG   334      39.264  87.104   2.308  1.00  0.00      A
ATOM   1826 HH12 ARG   334      39.849  87.584   3.865  1.00  0.00      A
ATOM   1827  NH2 ARG   334      41.043  89.634   3.103  1.00 45.11      A
ATOM   1828 HH21 ARG   334      41.486  90.433   2.698  1.00  0.00      A
ATOM   1829 HH22 ARG   334      41.109  89.471   4.088  1.00  0.00      A
ATOM   1830  C   ARG   334      37.846  87.374  -4.448  1.00 44.22      A
ATOM   1831  O   ARG   334      38.181  86.231  -4.788  1.00 40.32      A
ATOM   1832  N   ILE   335      36.662  87.903  -4.748  1.00 44.23      A
ATOM   1833  H   ILE   335      36.458  88.813  -4.452  1.00  0.00      A
```

ATOM	1834	CA	ILE	335	35.663	87.164	-5.504	1.00	45.07	A
ATOM	1835	CB	ILE	335	34.260	87.798	-5.329	1.00	46.64	A
ATOM	1836	CG2	ILE	335	34.330	89.285	-5.585	1.00	50.46	A
ATOM	1837	CG1	ILE	335	33.254	87.149	-6.283	1.00	50.93	A
ATOM	1838	CD1	ILE	335	33.110	85.645	-6.114	1.00	53.73	A
ATOM	1839	C	ILE	335	36.045	87.134	-6.977	1.00	41.85	A
ATOM	1840	O	ILE	335	36.246	86.070	-7.547	1.00	44.44	A
ATOM	1841	N	PHE	336	36.159	88.304	-7.591	1.00	38.93	A
ATOM	1842	H	PHE	336	35.995	89.130	-7.093	1.00	0.00	A
ATOM	1843	CA	PHE	336	36.526	88.371	-8.994	1.00	40.81	A
ATOM	1844	CB	PHE	336	36.041	89.684	-9.590	1.00	34.92	A
ATOM	1845	CG	PHE	336	34.548	89.816	-9.618	1.00	30.97	A
ATOM	1846	CD1	PHE	336	33.895	90.694	-8.753	1.00	30.10	A
ATOM	1847	CD2	PHE	336	33.792	89.072	-10.513	1.00	29.08	A
ATOM	1848	CE1	PHE	336	32.513	90.821	-8.783	1.00	15.73	A
ATOM	1849	CE2	PHE	336	32.409	89.197	-10.548	1.00	19.75	A
ATOM	1850	CZ	PHE	336	31.772	90.078	-9.677	1.00	20.19	A
ATOM	1851	C	PHE	336	38.035	88.240	-9.188	1.00	41.18	A
ATOM	1852	O	PHE	336	38.463	88.145	-10.356	1.00	41.37	A
ATOM	1853	OT	PHE	336	38.771	88.233	-8.178	1.00	40.25	A
ATOM	1854	CB	ALA	145	27.124	80.130	34.005	1.00	39.54	B
ATOM	1855	C	ALA	145	25.323	81.127	32.585	1.00	38.62	B
ATOM	1856	O	ALA	145	24.364	80.726	33.254	1.00	37.41	B
ATOM	1857	HT1	ALA	145	26.147	82.508	34.837	1.00	0.00	B
ATOM	1858	HT2	ALA	145	26.612	83.408	33.474	1.00	0.00	B
ATOM	1859	N	ALA	145	26.822	82.567	34.050	1.00	42.77	B
ATOM	1860	HT3	ALA	145	27.790	82.642	34.428	1.00	0.00	B
ATOM	1861	CA	ALA	145	26.715	81.343	33.203	1.00	39.62	B
ATOM	1862	N	GLN	146	25.236	81.388	31.288	1.00	33.32	B
ATOM	1863	H	GLN	146	26.034	81.700	30.819	1.00	0.00	B
ATOM	1864	CA	GLN	146	24.004	81.230	30.537	1.00	31.87	B
ATOM	1865	CB	GLN	146	24.024	82.162	29.354	1.00	29.22	B
ATOM	1866	CG	GLN	146	23.274	83.421	29.543	1.00	34.86	B
ATOM	1867	CD	GLN	146	23.349	84.236	28.288	1.00	39.34	B
ATOM	1868	OE1	GLN	146	24.442	84.554	27.821	1.00	41.32	B
ATOM	1869	NE2	GLN	146	22.200	84.559	27.720	1.00	38.82	B
ATOM	1870	HE21	GLN	146	21.354	84.268	28.120	1.00	0.00	B
ATOM	1871	HE22	GLN	146	22.239	85.092	26.900	1.00	0.00	B
ATOM	1872	C	GLN	146	23.862	79.804	30.023	1.00	27.45	B
ATOM	1873	O	GLN	146	24.525	79.400	29.079	1.00	22.32	B
ATOM	1874	N	LEU	147	22.965	79.050	30.622	1.00	27.23	B
ATOM	1875	H	LEU	147	22.423	79.419	31.350	1.00	0.00	B
ATOM	1876	CA	LEU	147	22.776	77.675	30.211	1.00	28.64	B
ATOM	1877	CB	LEU	147	23.538	76.760	31.165	1.00	27.79	B
ATOM	1878	CG	LEU	147	24.667	75.818	30.759	1.00	27.05	B
ATOM	1879	CD1	LEU	147	25.208	76.106	29.374	1.00	24.90	B
ATOM	1880	CD2	LEU	147	25.742	75.956	31.812	1.00	24.14	B
ATOM	1881	C	LEU	147	21.302	77.303	30.261	1.00	28.16	B
ATOM	1882	O	LEU	147	20.576	77.731	31.150	1.00	25.85	B
ATOM	1883	N	ASP	148	20.872	76.502	29.297	1.00	27.82	B
ATOM	1884	H	ASP	148	21.489	76.235	28.585	1.00	0.00	B
ATOM	1885	CA	ASP	148	19.506	76.019	29.279	1.00	22.46	B
ATOM	1886	CB	ASP	148	18.920	76.112	27.881	1.00	20.10	B
ATOM	1887	CG	ASP	148	18.424	77.504	27.561	1.00	12.21	B
ATOM	1888	OD1	ASP	148	18.422	77.881	26.375	1.00	14.78	B
ATOM	1889	OD2	ASP	148	18.040	78.216	28.494	1.00	13.58	B
ATOM	1890	C	ASP	148	19.703	74.568	29.680	1.00	21.73	B
ATOM	1891	O	ASP	148	20.389	73.822	28.986	1.00	23.66	B
ATOM	1892	N	ILE	149	19.138	74.190	30.822	1.00	17.82	B
ATOM	1893	H	ILE	149	18.603	74.833	31.327	1.00	0.00	B
ATOM	1894	CA	ILE	149	19.296	72.838	31.332	1.00	14.75	B
ATOM	1895	CB	ILE	149	19.901	72.847	32.752	1.00	15.94	B
ATOM	1896	CG2	ILE	149	20.143	71.431	33.218	1.00	8.68	B
ATOM	1897	CG1	ILE	149	21.192	73.685	32.788	1.00	13.92	B
ATOM	1898	CD1	ILE	149	21.672	73.954	34.217	1.00	7.01	B
ATOM	1899	C	ILE	149	17.977	72.076	31.427	1.00	19.66	B
ATOM	1900	O	ILE	149	16.969	72.581	31.935	1.00	17.11	B
ATOM	1901	N	VAL	150	18.008	70.843	30.959	1.00	15.39	B
ATOM	1902	H	VAL	150	18.833	70.497	30.565	1.00	0.00	B
ATOM	1903	CA	VAL	150	16.847	69.992	31.017	1.00	14.24	B
ATOM	1904	CB	VAL	150	16.399	69.565	29.612	1.00	18.62	B
ATOM	1905	CG1	VAL	150	15.323	68.478	29.707	1.00	11.48	B
ATOM	1906	CG2	VAL	150	15.861	70.773	28.869	1.00	14.10	B

	ATOM	1907	C	VAL	150	17.193	68.760	31.837	1.00	13.47	B
	ATOM	1908	O	VAL	150	18.166	68.050	31.558	1.00	16.28	B
	ATOM	1909	N	ILE	151	16.390	68.534	32.864	1.00	13.89	B
	ATOM	1910	H	ILE	151	15.666	69.164	33.048	1.00	0.00	B
5	ATOM	1911	CA	ILE	151	16.554	67.384	33.725	1.00	12.32	B
	ATOM	1912	CB	ILE	151	16.146	67.712	35.160	1.00	8.15	B
	ATOM	1913	CG2	ILE	151	16.359	66.524	36.033	1.00	4.81	B
	ATOM	1914	CG1	ILE	151	16.907	68.934	35.668	1.00	15.50	B
	ATOM	1915	CD1	ILE	151	16.390	69.451	37.017	1.00	16.51	B
10	ATOM	1916	C	ILE	151	15.625	66.309	33.174	1.00	12.57	B
	ATOM	1917	O	ILE	151	14.448	66.548	32.988	1.00	15.95	B
	ATOM	1918	N	VAL	152	16.184	65.141	32.869	1.00	16.00	B
	ATOM	1919	H	VAL	152	17.150	65.032	32.993	1.00	0.00	B
	ATOM	1920	CA	VAL	152	15.410	64.009	32.354	1.00	14.98	B
15	ATOM	1921	CB	VAL	152	16.082	63.397	31.106	1.00	15.24	B
	ATOM	1922	CG1	VAL	152	15.209	62.279	30.531	1.00	10.15	B
	ATOM	1923	CG2	VAL	152	16.313	64.500	30.056	1.00	7.29	B
	ATOM	1924	C	VAL	152	15.438	63.052	33.532	1.00	19.19	B
	ATOM	1925	O	VAL	152	16.459	62.414	33.835	1.00	16.07	B
20	ATOM	1926	N	LEU	153	14.297	62.976	34.200	1.00	15.97	B
	ATOM	1927	H	LEU	153	13.519	63.456	33.851	1.00	0.00	B
	ATOM	1928	CA	LEU	153	14.150	62.211	35.414	1.00	13.99	B
	ATOM	1929	CB	LEU	153	13.530	63.131	36.474	1.00	15.97	B
	ATOM	1930	CG	LEU	153	12.764	62.553	37.658	1.00	17.17	B
25	ATOM	1931	CD1	LEU	153	13.616	61.536	38.376	1.00	23.41	B
	ATOM	1932	CD2	LEU	153	12.367	63.672	38.599	1.00	15.08	B
	ATOM	1933	C	LEU	153	13.362	60.924	35.309	1.00	17.91	B
	ATOM	1934	O	LEU	153	12.214	60.923	34.870	1.00	23.80	B
	ATOM	1935	N	ASP	154	14.002	59.832	35.723	1.00	19.62	B
30	ATOM	1936	H	ASP	154	14.918	59.927	36.051	1.00	0.00	B
	ATOM	1937	CA	ASP	154	13.397	58.504	35.709	1.00	19.43	B
	ATOM	1938	CB	ASP	154	14.461	57.432	35.966	1.00	17.84	B
	ATOM	1939	CG	ASP	154	13.912	56.021	35.831	1.00	27.80	B
	ATOM	1940	OD1	ASP	154	12.725	55.871	35.461	1.00	28.40	B
35	ATOM	1941	OD2	ASP	154	14.667	55.059	36.094	1.00	28.69	B
	ATOM	1942	C	ASP	154	12.351	58.419	36.804	1.00	18.93	B
	ATOM	1943	O	ASP	154	12.698	58.429	37.993	1.00	15.86	B
	ATOM	1944	N	GLY	155	11.080	58.328	36.407	1.00	18.75	B
	ATOM	1945	H	GLY	155	10.873	58.317	35.453	1.00	0.00	B
40	ATOM	1946	CA	GLY	155	10.012	58.247	37.382	1.00	15.14	B
	ATOM	1947	C	GLY	155	9.479	56.842	37.537	1.00	19.82	B
	ATOM	1948	O	GLY	155	8.308	56.668	37.882	1.00	14.58	B
	ATOM	1949	N	SER	156	10.342	55.854	37.280	1.00	18.73	B
	ATOM	1950	H	SER	156	11.250	56.096	37.000	1.00	0.00	B
45	ATOM	1951	CA	SER	156	10.008	54.434	37.396	1.00	17.78	B
	ATOM	1952	CB	SER	156	11.217	53.559	36.993	1.00	23.82	B
	ATOM	1953	OG	SER	156	12.195	53.479	38.040	1.00	34.45	B
	ATOM	1954	HG	SER	156	12.517	54.359	38.245	1.00	0.00	B
	ATOM	1955	C	SER	156	9.581	54.127	38.826	1.00	14.28	B
50	ATOM	1956	O	SER	156	9.531	55.014	39.675	1.00	16.84	B
	ATOM	1957	N	ASN	157	9.298	52.866	39.113	1.00	15.15	B
	ATOM	1958	H	ASN	157	9.411	52.173	38.428	1.00	0.00	B
	ATOM	1959	CA	ASN	157	8.820	52.507	40.443	1.00	13.34	B
	ATOM	1960	CB	ASN	157	7.869	51.305	40.353	1.00	16.24	B
55	ATOM	1961	CG	ASN	157	6.634	51.580	39.529	1.00	20.72	B
	ATOM	1962	OD1	ASN	157	5.997	50.643	39.036	1.00	27.20	B
	ATOM	1963	ND2	ASN	157	6.273	52.859	39.374	1.00	18.41	B
	ATOM	1964	HD21	ASN	157	6.805	53.570	39.787	1.00	0.00	B
	ATOM	1965	HD22	ASN	157	5.473	53.041	38.841	1.00	0.00	B
60	ATOM	1966	C	ASN	157	9.865	52.190	41.511	1.00	16.46	B
	ATOM	1967	O	ASN	157	9.517	52.117	42.693	1.00	20.71	B
	ATOM	1968	N	SER	158	11.127	52.030	41.132	1.00	15.18	B
	ATOM	1969	H	SER	158	11.384	52.156	40.196	1.00	0.00	B
	ATOM	1970	CA	SER	158	12.151	51.654	42.127	1.00	16.23	B
65	ATOM	1971	CB	SER	158	13.161	50.690	41.487	1.00	13.88	B
	ATOM	1972	OG	SER	158	13.678	51.221	40.296	1.00	15.34	B
	ATOM	1973	HG	SER	158	14.121	52.052	40.478	1.00	0.00	B
	ATOM	1974	C	SER	158	12.911	52.713	42.948	1.00	17.21	B
	ATOM	1975	O	SER	158	13.395	52.397	44.046	1.00	16.37	B
70	ATOM	1976	N	ILE	159	13.061	53.938	42.446	1.00	22.58	B
	ATOM	1977	H	ILE	159	12.726	54.145	41.550	1.00	0.00	B
	ATOM	1978	CA	ILE	159	13.733	54.975	43.241	1.00	22.49	B
	ATOM	1979	CB	ILE	159	13.674	56.360	42.566	1.00	24.48	B

ATOM	1980	CG2	ILE	159	14.718	57.288	43.176	1.00	24.15	B
ATOM	1981	CG1	ILE	159	13.812	56.209	41.057	1.00	32.59	B
ATOM	1982	CD1	ILE	159	12.470	56.393	40.303	1.00	20.06	B
ATOM	1983	C	ILE	159	12.778	55.028	44.407	1.00	24.33	B
ATOM	1984	O	ILE	159	11.724	55.618	44.285	1.00	17.55	B
ATOM	1985	N	TYR	160	13.099	54.420	45.541	1.00	32.15	B
ATOM	1986	H	TYR	160	13.965	53.980	45.664	1.00	0.00	B
ATOM	1987	CA	TYR	160	12.097	54.447	46.585	1.00	31.82	B
ATOM	1988	CB	TYR	160	12.267	53.324	47.597	1.00	26.96	B
ATOM	1989	CG	TYR	160	11.253	53.490	48.725	1.00	25.65	B
ATOM	1990	CD1	TYR	160	9.926	53.897	48.457	1.00	24.26	B
ATOM	1991	CE1	TYR	160	9.022	54.114	49.484	1.00	18.27	B
ATOM	1992	CD2	TYR	160	11.623	53.306	50.041	1.00	20.35	B
ATOM	1993	CE2	TYR	160	10.729	53.519	51.072	1.00	22.84	B
ATOM	1994	CZ	TYR	160	9.441	53.917	50.791	1.00	14.51	B
ATOM	1995	OH	TYR	160	8.598	54.099	51.840	1.00	23.91	B
ATOM	1996	HH	TYR	160	9.063	53.916	52.661	1.00	0.00	B
ATOM	1997	C	TYR	160	11.880	55.733	47.356	1.00	37.48	B
ATOM	1998	O	TYR	160	10.799	56.335	47.262	1.00	44.11	B
ATOM	1999	N	PRO	161	12.855	56.167	48.158	1.00	31.96	B
ATOM	2000	CD	PRO	161	14.215	55.743	48.529	1.00	22.44	B
ATOM	2001	CA	PRO	161	12.466	57.408	48.822	1.00	28.82	B
ATOM	2002	CB	PRO	161	13.575	57.639	49.856	1.00	31.11	B
ATOM	2003	CG	PRO	161	14.337	56.332	49.902	1.00	29.58	B
ATOM	2004	C	PRO	161	12.414	58.464	47.729	1.00	23.46	B
ATOM	2005	O	PRO	161	13.452	58.977	47.298	1.00	18.53	B
ATOM	2006	N	TRP	162	11.204	58.741	47.246	1.00	23.04	B
ATOM	2007	H	TRP	162	10.424	58.275	47.612	1.00	0.00	B
ATOM	2008	CA	TRP	162	11.019	59.719	46.184	1.00	20.85	B
ATOM	2009	CB	TRP	162	9.565	59.743	45.720	1.00	24.84	B
ATOM	2010	CG	TRP	162	9.344	60.700	44.583	1.00	15.34	B
ATOM	2011	CD2	TRP	162	9.779	60.531	43.229	1.00	17.68	B
ATOM	2012	CE2	TRP	162	9.364	61.679	42.516	1.00	13.50	B
ATOM	2013	CE3	TRP	162	10.474	59.531	42.545	1.00	12.30	B
ATOM	2014	CD1	TRP	162	8.704	61.897	44.640	1.00	12.84	B
ATOM	2015	NE1	TRP	162	8.712	62.491	43.399	1.00	14.37	B
ATOM	2016	HE1	TRP	162	8.323	63.357	43.175	1.00	0.00	B
ATOM	2017	CZ2	TRP	162	9.625	61.847	41.158	1.00	14.57	B
ATOM	2018	CZ3	TRP	162	10.732	59.699	41.198	1.00	13.59	B
ATOM	2019	CH2	TRP	162	10.307	60.853	40.517	1.00	10.94	B
ATOM	2020	C	TRP	162	11.431	61.091	46.692	1.00	21.81	B
ATOM	2021	O	TRP	162	12.010	61.884	45.969	1.00	16.84	B
ATOM	2022	N	GLU	163	11.135	61.363	47.952	1.00	25.91	B
ATOM	2023	H	GLU	163	10.665	60.699	48.497	1.00	0.00	B
ATOM	2024	CA	GLU	163	11.506	62.644	48.524	1.00	33.12	B
ATOM	2025	CB	GLU	163	11.066	62.721	49.993	1.00	36.71	B
ATOM	2026	CG	GLU	163	11.646	61.637	50.888	1.00	47.66	B
ATOM	2027	CD	GLU	163	10.848	61.447	52.173	1.00	55.21	B
ATOM	2028	OE1	GLU	163	11.446	61.522	53.270	1.00	57.76	B
ATOM	2029	OE2	GLU	163	9.620	61.221	52.088	1.00	59.92	B
ATOM	2030	C	GLU	163	13.013	62.848	48.418	1.00	31.56	B
ATOM	2031	O	GLU	163	13.496	63.980	48.447	1.00	28.76	B
ATOM	2032	N	SER	164	13.748	61.747	48.270	1.00	31.75	B
ATOM	2033	H	SER	164	13.295	60.879	48.215	1.00	0.00	B
ATOM	2034	CA	SER	164	15.213	61.788	48.181	1.00	31.88	B
ATOM	2035	CB	SER	164	15.795	60.399	48.470	1.00	31.21	B
ATOM	2036	OG	SER	164	15.996	60.221	49.864	1.00	32.68	B
ATOM	2037	HG	SER	164	16.606	60.887	50.185	1.00	0.00	B
ATOM	2038	C	SER	164	15.751	62.289	46.845	1.00	29.05	B
ATOM	2039	O	SER	164	16.820	62.890	46.782	1.00	29.91	B
ATOM	2040	N	VAL	165	15.030	61.998	45.772	1.00	22.58	B
ATOM	2041	H	VAL	165	14.209	61.472	45.867	1.00	0.00	B
ATOM	2042	CA	VAL	165	15.443	62.454	44.462	1.00	26.86	B
ATOM	2043	CB	VAL	165	14.761	61.610	43.333	1.00	30.69	B
ATOM	2044	CG1	VAL	165	13.791	62.460	42.533	1.00	27.74	B
ATOM	2045	CG2	VAL	165	15.825	61.022	42.411	1.00	33.05	B
ATOM	2046	C	VAL	165	15.029	63.926	44.386	1.00	27.11	B
ATOM	2047	O	VAL	165	15.746	64.762	43.843	1.00	23.73	B
ATOM	2048	N	ILE	166	13.860	64.238	44.936	1.00	26.45	B
ATOM	2049	H	ILE	166	13.308	63.536	45.338	1.00	0.00	B
ATOM	2050	CA	ILE	166	13.388	65.618	44.943	1.00	21.89	B
ATOM	2051	CB	ILE	166	11.931	65.706	45.407	1.00	24.39	B
ATOM	2052	CG2	ILE	166	11.469	67.157	45.379	1.00	22.62	B

	ATOM	2053	CG1	ILE	166	11.047	64.822	44.505	1.00	28.66	B
	ATOM	2054	CD1	ILE	166	11.350	64.929	42.999	1.00	20.77	B
	ATOM	2055	C	ILE	166	14.283	66.471	45.842	1.00	18.82	B
	ATOM	2056	O	ILE	166	14.476	67.651	45.577	1.00	18.46	B
5	ATOM	2057	N	ALA	167	14.828	65.882	46.904	1.00	12.61	B
	ATOM	2058	H	ALA	167	14.615	64.949	47.105	1.00	0.00	B
	ATOM	2059	CA	ALA	167	15.750	66.625	47.768	1.00	14.63	B
	ATOM	2060	CB	ALA	167	16.054	65.836	49.048	1.00	15.91	B
	ATOM	2061	C	ALA	167	17.045	66.847	46.961	1.00	15.69	B
10	ATOM	2062	O	ALA	167	17.647	67.906	47.036	1.00	17.79	B
	ATOM	2063	N	PHE	168	17.450	65.842	46.181	1.00	14.44	B
	ATOM	2064	H	PHE	168	16.926	65.014	46.166	1.00	0.00	B
	ATOM	2065	CA	PHE	168	18.656	65.936	45.346	1.00	14.68	B
	ATOM	2066	CB	PHE	168	18.878	64.608	44.615	1.00	12.59	B
15	ATOM	2067	CG	PHE	168	19.832	64.680	43.444	1.00	20.18	B
	ATOM	2068	CD1	PHE	168	19.355	64.609	42.134	1.00	17.37	B
	ATOM	2069	CD2	PHE	168	21.211	64.759	43.645	1.00	16.50	B
	ATOM	2070	CE1	PHE	168	20.226	64.606	41.047	1.00	18.84	B
	ATOM	2071	CE2	PHE	168	22.092	64.760	42.564	1.00	14.29	B
20	ATOM	2072	CZ	PHE	168	21.599	64.680	41.263	1.00	15.75	B
	ATOM	2073	C	PHE	168	18.501	67.066	44.336	1.00	17.90	B
	ATOM	2074	O	PHE	168	19.420	67.847	44.114	1.00	19.14	B
	ATOM	2075	N	LEU	169	17.328	67.148	43.719	1.00	18.88	B
	ATOM	2076	H	LEU	169	16.627	66.494	43.929	1.00	0.00	B
25	ATOM	2077	CA	LEU	169	17.068	68.187	42.745	1.00	16.96	B
	ATOM	2078	CB	LEU	169	15.779	67.885	41.984	1.00	19.20	B
	ATOM	2079	CG	LEU	169	15.843	66.692	41.022	1.00	14.34	B
	ATOM	2080	CD1	LEU	169	14.476	66.482	40.428	1.00	16.09	B
	ATOM	2081	CD2	LEU	169	16.864	66.920	39.926	1.00	14.01	B
30	ATOM	2082	C	LEU	169	16.977	69.558	43.407	1.00	19.79	B
	ATOM	2083	O	LEU	169	17.443	70.547	42.844	1.00	26.07	B
	ATOM	2084	N	ASN	170	16.377	69.617	44.593	1.00	21.05	B
	ATOM	2085	H	ASN	170	16.011	68.795	44.984	1.00	0.00	B
	ATOM	2086	CA	ASN	170	16.249	70.875	45.332	1.00	22.16	B
35	ATOM	2087	CB	ASN	170	15.473	70.655	46.630	1.00	27.93	B
	ATOM	2088	CG	ASN	170	15.617	71.834	47.611	1.00	32.39	B
	ATOM	2089	OD1	ASN	170	16.661	72.003	48.257	1.00	29.22	B
	ATOM	2090	ND2	ASN	170	14.572	72.643	47.718	1.00	25.77	B
	ATOM	2091	HD21	ASN	170	13.765	72.473	47.191	1.00	0.00	B
40	ATOM	2092	HD22	ASN	170	14.648	73.396	48.340	1.00	0.00	B
	ATOM	2093	C	ASN	170	17.609	71.498	45.668	1.00	24.44	B
	ATOM	2094	O	ASN	170	17.832	72.689	45.426	1.00	24.64	B
	ATOM	2095	N	ASP	171	18.509	70.684	46.223	1.00	22.99	B
	ATOM	2096	H	ASP	171	18.262	69.748	46.378	1.00	0.00	B
45	ATOM	2097	CA	ASP	171	19.855	71.128	46.610	1.00	20.63	B
	ATOM	2098	CB	ASP	171	20.593	70.014	47.360	1.00	20.85	B
	ATOM	2099	CG	ASP	171	19.869	69.585	48.619	1.00	29.81	B
	ATOM	2100	OD1	ASP	171	19.031	70.371	49.124	1.00	25.40	B
	ATOM	2101	OD2	ASP	171	20.131	68.465	49.104	1.00	29.96	B
50	ATOM	2102	C	ASP	171	20.685	71.544	45.416	1.00	22.06	B
	ATOM	2103	O	ASP	171	21.537	72.431	45.519	1.00	26.11	B
	ATOM	2104	N	LEU	172	20.447	70.876	44.292	1.00	19.55	B
	ATOM	2105	H	LEU	172	19.776	70.165	44.301	1.00	0.00	B
	ATOM	2106	CA	LEU	172	21.146	71.162	43.050	1.00	20.55	B
55	ATOM	2107	CB	LEU	172	20.866	70.044	42.056	1.00	25.39	B
	ATOM	2108	CG	LEU	172	21.889	69.703	40.978	1.00	23.87	B
	ATOM	2109	CD1	LEU	172	21.174	68.935	39.874	1.00	26.42	B
	ATOM	2110	CD2	LEU	172	22.543	70.947	40.435	1.00	32.73	B
	ATOM	2111	C	LEU	172	20.697	72.484	42.428	1.00	20.44	B
60	ATOM	2112	O	LEU	172	21.518	73.313	42.014	1.00	21.12	B
	ATOM	2113	N	LEU	173	19.383	72.646	42.343	1.00	18.93	B
	ATOM	2114	H	LEU	173	18.803	71.938	42.694	1.00	0.00	B
	ATOM	2115	CA	LEU	173	18.761	73.826	41.755	1.00	21.30	B
	ATOM	2116	CB	LEU	173	17.248	73.588	41.573	1.00	20.45	B
65	ATOM	2117	CG	LEU	173	16.850	72.431	40.649	1.00	20.49	B
	ATOM	2118	CD1	LEU	173	15.418	72.019	40.926	1.00	22.02	B
	ATOM	2119	CD2	LEU	173	16.999	72.855	39.197	1.00	25.70	B
	ATOM	2120	C	LEU	173	18.966	75.081	42.583	1.00	18.86	B
	ATOM	2121	O	LEU	173	19.266	76.146	42.046	1.00	16.41	B
70	ATOM	2122	N	LYS	174	18.799	74.953	43.894	1.00	21.55	B
	ATOM	2123	H	LYS	174	18.581	74.076	44.275	1.00	0.00	B
	ATOM	2124	CA	LYS	174	18.943	76.107	44.765	1.00	23.18	B
	ATOM	2125	CB	LYS	174	18.648	75.717	46.216	1.00	26.28	B

ATOM	2126	CG	LYS	174	19.830	75.202	47.026	1.00	29.25	B
ATOM	2127	CD	LYS	174	19.306	74.550	48.304	1.00	28.29	B
ATOM	2128	CE	LYS	174	20.399	73.886	49.111	1.00	19.54	B
ATOM	2129	NZ	LYS	174	19.815	73.374	50.359	1.00	21.14	B
ATOM	2130	HZ1	LYS	174	19.069	72.682	50.131	1.00	0.00	B
ATOM	2131	HZ2	LYS	174	19.398	74.161	50.895	1.00	0.00	B
ATOM	2132	HZ3	LYS	174	20.551	72.915	50.926	1.00	0.00	B
ATOM	2133	C	LYS	174	20.288	76.818	44.661	1.00	22.91	B
ATOM	2134	O	LYS	174	20.420	77.948	45.110	1.00	22.73	B
ATOM	2135	N	ALA	175	21.279	76.173	44.059	1.00	23.45	B
ATOM	2136	H	ALA	175	21.134	75.270	43.705	1.00	0.00	B
ATOM	2137	CA	ALA	175	22.589	76.807	43.929	1.00	26.35	B
ATOM	2138	CB	ALA	175	23.694	75.755	43.981	1.00	22.79	B
ATOM	2139	C	ALA	175	22.730	77.649	42.658	1.00	26.76	B
ATOM	2140	O	ALA	175	23.651	78.460	42.539	1.00	29.91	B
ATOM	2141	N	MET	176	21.821	77.470	41.710	1.00	25.18	B
ATOM	2142	H	MET	176	21.098	76.822	41.845	1.00	0.00	B
ATOM	2143	CA	MET	176	21.888	78.226	40.467	1.00	24.53	B
ATOM	2144	CB	MET	176	21.253	77.418	39.336	1.00	22.97	B
ATOM	2145	CG	MET	176	21.779	76.003	39.265	1.00	22.20	B
ATOM	2146	SD	MET	176	20.923	74.945	38.090	1.00	24.68	B
ATOM	2147	CE	MET	176	22.045	73.494	38.136	1.00	19.10	B
ATOM	2148	C	MET	176	21.227	79.595	40.548	1.00	24.31	B
ATOM	2149	O	MET	176	20.618	79.958	41.554	1.00	31.33	B
ATOM	2150	N	ASP	177	21.365	80.354	39.469	1.00	24.61	B
ATOM	2151	H	ASP	177	21.887	80.004	38.717	1.00	0.00	B
ATOM	2152	CA	ASP	177	20.777	81.678	39.355	1.00	24.49	B
ATOM	2153	CB	ASP	177	21.848	82.729	39.075	1.00	30.14	B
ATOM	2154	CG	ASP	177	21.348	84.131	39.296	1.00	33.29	B
ATOM	2155	OD1	ASP	177	22.134	84.977	39.767	1.00	37.03	B
ATOM	2156	OD2	ASP	177	20.160	84.388	39.000	1.00	42.39	B
ATOM	2157	C	ASP	177	19.881	81.525	38.153	1.00	21.41	B
ATOM	2158	O	ASP	177	20.365	81.519	37.017	1.00	20.00	B
ATOM	2159	N	ILE	178	18.581	81.390	38.407	1.00	18.68	B
ATOM	2160	H	ILE	178	18.270	81.436	39.336	1.00	0.00	B
ATOM	2161	CA	ILE	178	17.610	81.169	37.350	1.00	20.35	B
ATOM	2162	CB	ILE	178	16.525	80.193	37.788	1.00	24.17	B
ATOM	2163	CG2	ILE	178	15.745	79.714	36.559	1.00	26.64	B
ATOM	2164	CG1	ILE	178	17.154	79.024	38.560	1.00	26.03	B
ATOM	2165	CD1	ILE	178	17.407	77.790	37.734	1.00	21.54	B
ATOM	2166	C	ILE	178	16.916	82.410	36.840	1.00	21.48	B
ATOM	2167	O	ILE	178	16.327	83.164	37.598	1.00	13.16	B
ATOM	2168	N	GLY	179	16.977	82.586	35.527	1.00	23.27	B
ATOM	2169	H	GLY	179	17.457	81.937	34.974	1.00	0.00	B
ATOM	2170	CA	GLY	179	16.346	83.727	34.904	1.00	24.96	B
ATOM	2171	C	GLY	179	16.621	83.775	33.414	1.00	25.44	B
ATOM	2172	O	GLY	179	17.505	83.087	32.906	1.00	18.86	B
ATOM	2173	N	PRO	180	15.844	84.583	32.685	1.00	27.50	B
ATOM	2174	CD	PRO	180	14.721	85.395	33.194	1.00	23.45	B
ATOM	2175	CA	PRO	180	16.006	84.725	31.240	1.00	25.34	B
ATOM	2176	CB	PRO	180	14.991	85.817	30.881	1.00	28.96	B
ATOM	2177	CG	PRO	180	13.934	85.689	31.956	1.00	21.85	B
ATOM	2178	C	PRO	180	17.434	85.104	30.859	1.00	21.40	B
ATOM	2179	O	PRO	180	17.889	84.771	29.780	1.00	17.19	B
ATOM	2180	N	LYS	181	18.126	85.779	31.773	1.00	22.62	B
ATOM	2181	H	LYS	181	17.698	85.977	32.631	1.00	0.00	B
ATOM	2182	CA	LYS	181	19.493	86.244	31.555	1.00	22.16	B
ATOM	2183	CB	LYS	181	19.628	87.682	32.050	1.00	27.02	B
ATOM	2184	CG	LYS	181	18.711	88.652	31.352	1.00	32.06	B
ATOM	2185	CD	LYS	181	19.157	88.876	29.925	1.00	29.94	B
ATOM	2186	CE	LYS	181	19.909	90.182	29.788	1.00	34.20	B
ATOM	2187	NZ	LYS	181	20.167	90.503	28.357	1.00	34.68	B
ATOM	2188	HZ1	LYS	181	19.264	90.584	27.850	1.00	0.00	B
ATOM	2189	HZ2	LYS	181	20.738	89.744	27.930	1.00	0.00	B
ATOM	2190	HZ3	LYS	181	20.685	91.402	28.291	1.00	0.00	B
ATOM	2191	C	LYS	181	20.585	85.395	32.206	1.00	22.21	B
ATOM	2192	O	LYS	181	21.764	85.684	32.044	1.00	20.87	B
ATOM	2193	N	GLN	182	20.194	84.379	32.958	1.00	23.88	B
ATOM	2194	H	GLN	182	19.235	84.212	33.077	1.00	0.00	B
ATOM	2195	CA	GLN	182	21.156	83.498	33.616	1.00	27.46	B
ATOM	2196	CB	GLN	182	21.004	83.585	35.136	1.00	31.07	B
ATOM	2197	CG	GLN	182	20.735	84.991	35.668	1.00	38.02	B
ATOM	2198	CD	GLN	182	21.886	85.950	35.421	1.00	42.63	B

	ATOM	2199	OE1	GLN	182	21.708	87.167	35.435	1.00	44.04	B
	ATOM	2200	NE2	GLN	182	23.072	85.406	35.190	1.00	43.73	B
	ATOM	2201	HE21	GLN	182	23.171	84.431	35.184	1.00	0.00	B
	ATOM	2202	HE22	GLN	182	23.824	86.012	35.029	1.00	0.00	B
	ATOM	2203	C	GLN	182	20.880	82.076	33.135	1.00	26.08	B
	ATOM	2204	O	GLN	182	20.806	81.835	31.926	1.00	22.28	B
	ATOM	2205	N	THR	183	20.732	81.132	34.058	1.00	18.41	B
	ATOM	2206	H	THR	183	20.823	81.350	35.010	1.00	0.00	B
	ATOM	2207	CA	THR	183	20.439	79.778	33.640	1.00	21.94	B
	ATOM	2208	CB	THR	183	21.165	78.705	34.513	1.00	27.45	B
	ATOM	2209	OG1	THR	183	20.203	77.844	35.121	1.00	36.22	B
	ATOM	2210	HG1	THR	183	19.691	77.402	34.438	1.00	0.00	B
	ATOM	2211	CG2	THR	183	22.028	79.347	35.563	1.00	20.20	B
	ATOM	2212	C	THR	183	18.936	79.531	33.646	1.00	18.10	B
	ATOM	2213	O	THR	183	18.178	80.193	34.360	1.00	19.07	B
	ATOM	2214	N	GLN	184	18.509	78.607	32.797	1.00	15.96	B
	ATOM	2215	H	GLN	184	19.158	78.154	32.225	1.00	0.00	B
	ATOM	2216	CA	GLN	184	17.107	78.245	32.693	1.00	16.73	B
	ATOM	2217	CB	GLN	184	16.564	78.600	31.305	1.00	20.17	B
	ATOM	2218	CG	GLN	184	16.243	80.079	31.118	1.00	15.38	B
	ATOM	2219	CD	GLN	184	15.181	80.307	30.063	1.00	14.63	B
	ATOM	2220	OE1	GLN	184	14.165	80.926	30.326	1.00	17.14	B
	ATOM	2221	NE2	GLN	184	15.416	79.801	28.859	1.00	17.84	B
	ATOM	2222	HE21	GLN	184	16.245	79.305	28.694	1.00	0.00	B
	ATOM	2223	HE22	GLN	184	14.737	79.942	28.172	1.00	0.00	B
	ATOM	2224	C	GLN	184	17.023	76.740	32.905	1.00	16.49	B
	ATOM	2225	O	GLN	184	17.841	75.981	32.377	1.00	18.75	B
	ATOM	2226	N	VAL	185	16.043	76.311	33.685	1.00	19.05	B
	ATOM	2227	H	VAL	185	15.437	76.962	34.095	1.00	0.00	B
	ATOM	2228	CA	VAL	185	15.849	74.895	33.943	1.00	15.68	B
	ATOM	2229	CB	VAL	185	16.145	74.549	35.437	1.00	15.74	B
	ATOM	2230	CG1	VAL	185	15.608	73.149	35.795	1.00	14.91	B
	ATOM	2231	CG2	VAL	185	17.641	74.610	35.686	1.00	13.27	B
	ATOM	2232	C	VAL	185	14.411	74.506	33.614	1.00	16.98	B
	ATOM	2233	O	VAL	185	13.458	75.230	33.923	1.00	17.38	B
	ATOM	2234	N	GLY	186	14.296	73.364	32.948	1.00	20.72	B
	ATOM	2235	H	GLY	186	15.109	72.886	32.688	1.00	0.00	B
	ATOM	2236	CA	GLY	186	13.016	72.794	32.585	1.00	14.37	B
	ATOM	2237	C	GLY	186	13.134	71.359	33.073	1.00	16.88	B
	ATOM	2238	O	GLY	186	14.252	70.825	33.165	1.00	10.74	B
	ATOM	2239	N	ILE	187	12.020	70.721	33.409	1.00	12.53	B
	ATOM	2240	H	ILE	187	11.152	71.172	33.346	1.00	0.00	B
	ATOM	2241	CA	ILE	187	12.104	69.344	33.869	1.00	14.75	B
	ATOM	2242	CB	ILE	187	11.766	69.193	35.366	1.00	9.81	B
	ATOM	2243	CG2	ILE	187	11.733	67.712	35.742	1.00	10.78	B
	ATOM	2244	CG1	ILE	187	12.818	69.901	36.207	1.00	10.95	B
	ATOM	2245	CD1	ILE	187	12.517	69.886	37.678	1.00	7.68	B
	ATOM	2246	C	ILE	187	11.191	68.422	33.105	1.00	12.90	B
	ATOM	2247	O	ILE	187	10.022	68.699	32.908	1.00	14.75	B
	ATOM	2248	N	VAL	188	11.756	67.299	32.696	1.00	20.73	B
	ATOM	2249	H	VAL	188	12.703	67.157	32.892	1.00	0.00	B
	ATOM	2250	CA	VAL	188	11.040	66.267	31.970	1.00	18.34	B
	ATOM	2251	CB	VAL	188	11.748	65.977	30.620	1.00	23.42	B
	ATOM	2252	CG1	VAL	188	11.363	64.610	30.107	1.00	17.83	B
	ATOM	2253	CG2	VAL	188	11.432	67.075	29.602	1.00	16.65	B
	ATOM	2254	C	VAL	188	11.077	64.992	32.831	1.00	22.16	B
	ATOM	2255	O	VAL	188	12.126	64.630	33.373	1.00	12.92	B
	ATOM	2256	N	GLN	189	9.929	64.338	33.014	1.00	19.46	B
	ATOM	2257	H	GLN	189	9.092	64.704	32.661	1.00	0.00	B
	ATOM	2258	CA	GLN	189	9.938	63.076	33.742	1.00	20.85	B
	ATOM	2259	CB	GLN	189	9.039	63.076	34.980	1.00	16.60	B
	ATOM	2260	CG	GLN	189	8.890	61.643	35.564	1.00	16.53	B
	ATOM	2261	CD	GLN	189	8.284	61.597	36.966	1.00	18.48	B
	ATOM	2262	OE1	GLN	189	8.274	60.553	37.608	1.00	17.85	B
	ATOM	2263	NE2	GLN	189	7.777	62.734	37.431	1.00	22.55	B
	ATOM	2264	HE21	GLN	189	7.800	63.546	36.889	1.00	0.00	B
	ATOM	2265	HE22	GLN	189	7.387	62.711	38.332	1.00	0.00	B
	ATOM	2266	C	GLN	189	9.444	62.015	32.769	1.00	18.02	B
	ATOM	2267	O	GLN	189	8.630	62.295	31.903	1.00	13.48	B
	ATOM	2268	N	TYR	190	9.963	60.799	32.897	1.00	17.53	B
	ATOM	2269	H	TYR	190	10.629	60.631	33.593	1.00	0.00	B
	ATOM	2270	CA	TYR	190	9.553	59.725	32.022	1.00	16.18	B
	ATOM	2271	CB	TYR	190	10.587	59.512	30.894	1.00	21.58	B

ATOM	2272	CG	TYR	190	11.882	58.859	31.318	1.00	24.13	B
ATOM	2273	CD1	TYR	190	12.035	57.474	31.253	1.00	29.37	B
ATOM	2274	CE1	TYR	190	13.194	56.859	31.702	1.00	26.64	B
ATOM	2275	CD2	TYR	190	12.937	59.617	31.835	1.00	22.88	B
ATOM	2276	CE2	TYR	190	14.105	59.006	32.283	1.00	22.43	B
ATOM	2277	CZ	TYR	190	14.220	57.632	32.221	1.00	24.14	B
ATOM	2278	OH	TYR	190	15.330	57.013	32.741	1.00	25.80	B
ATOM	2279	HH	TYR	190	15.251	56.064	32.618	1.00	0.00	B
ATOM	2280	C	TYR	190	9.346	58.474	32.860	1.00	17.06	B
ATOM	2281	O	TYR	190	9.753	58.408	34.027	1.00	19.81	B
ATOM	2282	N	GLY	191	8.666	57.502	32.273	1.00	18.92	B
ATOM	2283	H	GLY	191	8.353	57.624	31.354	1.00	0.00	B
ATOM	2284	CA	GLY	191	8.373	56.255	32.963	1.00	16.20	B
ATOM	2285	C	GLY	191	7.278	55.625	32.137	1.00	17.90	B
ATOM	2286	O	GLY	191	6.100	55.732	32.480	1.00	34.36	B
ATOM	2287	N	GLU	192	7.672	54.993	31.041	1.00	16.02	B
ATOM	2288	H	GLU	192	8.631	54.939	30.847	1.00	0.00	B
ATOM	2289	CA	GLU	192	6.728	54.371	30.100	1.00	24.28	B
ATOM	2290	CB	GLU	192	5.433	53.920	30.798	1.00	31.95	B
ATOM	2291	CG	GLU	192	5.253	52.419	30.945	1.00	36.40	B
ATOM	2292	CD	GLU	192	4.309	52.063	32.084	1.00	46.73	B
ATOM	2293	OE1	GLU	192	3.996	50.864	32.253	1.00	46.15	B
ATOM	2294	OE2	GLU	192	3.878	52.985	32.815	1.00	50.61	B
ATOM	2295	C	GLU	192	6.397	55.450	29.077	1.00	19.84	B
ATOM	2296	O	GLU	192	6.518	55.239	27.870	1.00	16.66	B
ATOM	2297	N	ASN	193	5.990	56.614	29.580	1.00	13.96	B
ATOM	2298	H	ASN	193	5.913	56.713	30.550	1.00	0.00	B
ATOM	2299	CA	ASN	193	5.659	57.750	28.722	1.00	18.10	B
ATOM	2300	CB	ASN	193	4.150	58.065	28.785	1.00	17.15	B
ATOM	2301	CG	ASN	193	3.290	56.962	28.183	1.00	17.46	B
ATOM	2302	OD1	ASN	193	3.165	56.857	26.965	1.00	24.21	B
ATOM	2303	ND2	ASN	193	2.690	56.138	29.040	1.00	9.82	B
ATOM	2304	HD21	ASN	193	2.815	56.262	30.004	1.00	0.00	B
ATOM	2305	HD22	ASN	193	2.135	55.426	28.665	1.00	0.00	B
ATOM	2306	C	ASN	193	6.468	58.961	29.202	1.00	16.97	B
ATOM	2307	O	ASN	193	7.080	58.918	30.280	1.00	19.37	B
ATOM	2308	N	VAL	194	6.470	60.025	28.404	1.00	13.36	B
ATOM	2309	H	VAL	194	5.964	59.992	27.567	1.00	0.00	B
ATOM	2310	CA	VAL	194	7.204	61.250	28.734	1.00	18.46	B
ATOM	2311	CB	VAL	194	8.117	61.699	27.555	1.00	17.45	B
ATOM	2312	CG1	VAL	194	9.043	62.818	28.003	1.00	16.70	B
ATOM	2313	CG2	VAL	194	8.901	60.526	27.022	1.00	11.05	B
ATOM	2314	C	VAL	194	6.284	62.417	29.047	1.00	18.32	B
ATOM	2315	O	VAL	194	5.377	62.710	28.273	1.00	17.95	B
ATOM	2316	N	THR	195	6.543	63.095	30.164	1.00	18.97	B
ATOM	2317	H	THR	195	7.285	62.797	30.728	1.00	0.00	B
ATOM	2318	CA	THR	195	5.768	64.265	30.582	1.00	20.52	B
ATOM	2319	CB	THR	195	5.012	63.982	31.906	1.00	18.21	B
ATOM	2320	OG1	THR	195	5.765	64.482	33.014	1.00	30.10	B
ATOM	2321	HG1	THR	195	5.291	64.302	33.830	1.00	0.00	B
ATOM	2322	CG2	THR	195	4.828	62.510	32.091	1.00	23.60	B
ATOM	2323	C	THR	195	6.673	65.486	30.791	1.00	24.72	B
ATOM	2324	O	THR	195	7.792	65.355	31.302	1.00	25.20	B
ATOM	2325	N	HIS	196	6.216	66.669	30.371	1.00	24.33	B
ATOM	2326	H	HIS	196	5.347	66.719	29.922	1.00	0.00	B
ATOM	2327	CA	HIS	196	6.997	67.890	30.576	1.00	20.06	B
ATOM	2328	CB	HIS	196	6.787	68.891	29.438	1.00	20.11	B
ATOM	2329	CG	HIS	196	7.414	68.468	28.144	1.00	31.04	B
ATOM	2330	CD2	HIS	196	6.916	67.757	27.103	1.00	32.61	B
ATOM	2331	ND1	HIS	196	8.723	68.754	27.823	1.00	32.93	B
ATOM	2332	HD1	HIS	196	9.343	69.258	28.384	1.00	0.00	B
ATOM	2333	CE1	HIS	196	9.008	68.235	26.640	1.00	30.15	B
ATOM	2334	NE2	HIS	196	7.929	67.625	26.183	1.00	29.88	B
ATOM	2335	HE2	HIS	196	7.865	67.157	25.331	1.00	0.00	B
ATOM	2336	C	HIS	196	6.449	68.473	31.864	1.00	23.53	B
ATOM	2337	O	HIS	196	5.330	68.968	31.872	1.00	24.48	B
ATOM	2338	N	GLU	197	7.214	68.392	32.959	1.00	21.43	B
ATOM	2339	H	GLU	197	8.101	67.980	32.898	1.00	0.00	B
ATOM	2340	CA	GLU	197	6.745	68.908	34.244	1.00	21.98	B
ATOM	2341	CB	GLU	197	7.635	68.416	35.385	1.00	22.07	B
ATOM	2342	CG	GLU	197	7.553	66.900	35.626	1.00	22.26	B
ATOM	2343	CD	GLU	197	6.265	66.461	36.330	1.00	19.16	B
ATOM	2344	OE1	GLU	197	5.436	67.324	36.655	1.00	21.45	B

ATOM	2345	OE2	GLU	197	6.080	65.252	36.559	1.00	25.81	B
ATOM	2346	C	GLU	197	6.697	70.432	34.179	1.00	21.01	B
ATOM	2347	O	GLU	197	5.771	71.057	34.704	1.00	20.20	B
ATOM	2348	N	PHE	198	7.715	71.028	33.568	1.00	20.63	B
ATOM	2349	H	PHE	198	8.475	70.486	33.270	1.00	0.00	B
ATOM	2350	CA	PHE	198	7.733	72.465	33.329	1.00	16.85	B
ATOM	2351	CB	PHE	198	7.846	73.321	34.618	1.00	19.79	B
ATOM	2352	CG	PHE	198	9.077	73.099	35.447	1.00	18.93	B
ATOM	2353	CD1	PHE	198	10.282	73.736	35.134	1.00	15.68	B
ATOM	2354	CD2	PHE	198	9.003	72.358	36.619	1.00	17.58	B
ATOM	2355	CE1	PHE	198	11.389	73.642	35.984	1.00	8.10	B
ATOM	2356	CE2	PHE	198	10.113	72.258	37.480	1.00	17.77	B
ATOM	2357	CZ	PHE	198	11.307	72.909	37.154	1.00	18.12	B
ATOM	2358	C	PHE	198	8.773	72.827	32.285	1.00	23.38	B
ATOM	2359	O	PHE	198	9.848	72.210	32.191	1.00	19.68	B
ATOM	2360	N	ASN	199	8.403	73.797	31.457	1.00	22.68	B
ATOM	2361	H	ASN	199	7.536	74.227	31.581	1.00	0.00	B
ATOM	2362	CA	ASN	199	9.251	74.241	30.379	1.00	19.07	B
ATOM	2363	CB	ASN	199	8.402	74.980	29.342	1.00	18.17	B
ATOM	2364	CG	ASN	199	7.545	74.033	28.511	1.00	16.13	B
ATOM	2365	OD1	ASN	199	7.520	72.824	28.741	1.00	21.16	B
ATOM	2366	ND2	ASN	199	6.849	74.579	27.532	1.00	18.89	B
ATOM	2367	HD21	ASN	199	6.902	75.547	27.376	1.00	0.00	B
ATOM	2368	HD22	ASN	199	6.292	73.989	26.986	1.00	0.00	B
ATOM	2369	C	ASN	199	10.434	75.094	30.832	1.00	15.04	B
ATOM	2370	O	ASN	199	10.465	75.613	31.944	1.00	15.97	B
ATOM	2371	N	LEU	200	11.414	75.189	29.935	1.00	20.27	B
ATOM	2372	H	LEU	200	11.297	74.727	29.080	1.00	0.00	B
ATOM	2373	CA	LEU	200	12.655	75.939	30.140	1.00	20.09	B
ATOM	2374	CB	LEU	200	13.504	75.847	28.859	1.00	20.33	B
ATOM	2375	CG	LEU	200	15.000	75.481	28.771	1.00	19.69	B
ATOM	2376	CD1	LEU	200	15.510	74.719	29.975	1.00	14.91	B
ATOM	2377	CD2	LEU	200	15.189	74.680	27.506	1.00	11.40	B
ATOM	2378	C	LEU	200	12.387	77.404	30.468	1.00	18.48	B
ATOM	2379	O	LEU	200	13.155	78.034	31.193	1.00	20.99	B
ATOM	2380	N	ASN	201	11.295	77.949	29.940	1.00	13.45	B
ATOM	2381	H	ASN	201	10.701	77.403	29.382	1.00	0.00	B
ATOM	2382	CA	ASN	201	10.978	79.350	30.190	1.00	22.91	B
ATOM	2383	CB	ASN	201	10.645	80.061	28.877	1.00	23.93	B
ATOM	2384	CG	ASN	201	9.360	79.545	28.229	1.00	25.62	B
ATOM	2385	OD1	ASN	201	9.048	79.911	27.103	1.00	32.16	B
ATOM	2386	ND2	ASN	201	8.624	78.700	28.932	1.00	24.92	B
ATOM	2387	HD21	ASN	201	8.908	78.429	29.828	1.00	0.00	B
ATOM	2388	HD22	ASN	201	7.801	78.368	28.519	1.00	0.00	B
ATOM	2389	C	ASN	201	9.826	79.549	31.162	1.00	24.74	B
ATOM	2390	O	ASN	201	9.352	80.664	31.329	1.00	21.95	B
ATOM	2391	N	LYS	202	9.378	78.468	31.789	1.00	27.24	B
ATOM	2392	H	LYS	202	9.806	77.604	31.615	1.00	0.00	B
ATOM	2393	CA	LYS	202	8.261	78.527	32.735	1.00	28.50	B
ATOM	2394	CB	LYS	202	7.936	77.122	33.249	1.00	35.35	B
ATOM	2395	CG	LYS	202	6.537	77.001	33.861	1.00	44.45	B
ATOM	2396	CD	LYS	202	5.511	76.529	32.828	1.00	51.43	B
ATOM	2397	CE	LYS	202	5.819	75.112	32.334	1.00	52.91	B
ATOM	2398	NZ	LYS	202	5.156	74.748	31.049	1.00	49.04	B
ATOM	2399	HZ1	LYS	202	5.462	75.400	30.301	1.00	0.00	B
ATOM	2400	HZ2	LYS	202	4.124	74.807	31.163	1.00	0.00	B
ATOM	2401	HZ3	LYS	202	5.419	73.774	30.788	1.00	0.00	B
ATOM	2402	C	LYS	202	8.450	79.451	33.934	1.00	25.89	B
ATOM	2403	O	LYS	202	7.550	80.227	34.260	1.00	25.05	B
ATOM	2404	N	TYR	203	9.617	79.348	34.577	1.00	22.72	B
ATOM	2405	H	TYR	203	10.276	78.722	34.225	1.00	0.00	B
ATOM	2406	CA	TYR	203	9.978	80.123	35.770	1.00	26.57	B
ATOM	2407	CB	TYR	203	10.246	79.166	36.937	1.00	20.51	B
ATOM	2408	CG	TYR	203	9.065	78.303	37.215	1.00	23.59	B
ATOM	2409	CD1	TYR	203	9.075	76.941	36.901	1.00	24.81	B
ATOM	2410	CE1	TYR	203	7.927	76.163	37.057	1.00	23.81	B
ATOM	2411	CD2	TYR	203	7.886	78.870	37.706	1.00	26.42	B
ATOM	2412	CE2	TYR	203	6.741	78.113	37.871	1.00	28.83	B
ATOM	2413	CZ	TYR	203	6.762	76.763	37.542	1.00	32.83	B
ATOM	2414	OH	TYR	203	5.598	76.043	37.683	1.00	29.24	B
ATOM	2415	HH	TYR	203	5.758	75.133	37.423	1.00	0.00	B
ATOM	2416	C	TYR	203	11.201	81.013	35.569	1.00	27.09	B
ATOM	2417	O	TYR	203	12.229	80.563	35.056	1.00	24.90	B

ATOM	2418	N	SER	204	11.089	82.268	35.995	1.00	29.38	B
ATOM	2419	H	SER	204	10.256	82.561	36.419	1.00	0.00	B
ATOM	2420	CA	SER	204	12.189	83.216	35.845	1.00	29.68	B
ATOM	2421	CB	SER	204	11.701	84.509	35.158	1.00	29.69	B
ATOM	2422	OG	SER	204	10.458	84.974	35.668	1.00	34.41	B
ATOM	2423	HG	SER	204	9.786	84.301	35.536	1.00	0.00	B
ATOM	2424	C	SER	204	12.917	83.547	37.150	1.00	30.79	B
ATOM	2425	O	SER	204	13.453	84.642	37.314	1.00	31.71	B
ATOM	2426	N	SER	205	12.934	82.587	38.074	1.00	28.19	B
ATOM	2427	H	SER	205	12.458	81.749	37.903	1.00	0.00	B
ATOM	2428	CA	SER	205	13.642	82.755	39.334	1.00	22.80	B
ATOM	2429	CB	SER	205	12.895	83.709	40.263	1.00	23.08	B
ATOM	2430	OG	SER	205	11.998	83.004	41.097	1.00	23.87	B
ATOM	2431	HG	SER	205	11.543	83.623	41.672	1.00	0.00	B
ATOM	2432	C	SER	205	13.851	81.395	40.003	1.00	25.18	B
ATOM	2433	O	SER	205	13.079	80.451	39.794	1.00	20.34	B
ATOM	2434	N	THR	206	14.919	81.307	40.788	1.00	23.66	B
ATOM	2435	H	THR	206	15.486	82.100	40.902	1.00	0.00	B
ATOM	2436	CA	THR	206	15.289	80.086	41.487	1.00	27.98	B
ATOM	2437	CB	THR	206	16.678	80.229	42.129	1.00	26.89	B
ATOM	2438	OG1	THR	206	17.514	81.019	41.272	1.00	29.58	B
ATOM	2439	HG1	THR	206	17.597	80.587	40.418	1.00	0.00	B
ATOM	2440	CG2	THR	206	17.319	78.875	42.330	1.00	22.76	B
ATOM	2441	C	THR	206	14.295	79.661	42.556	1.00	29.88	B
ATOM	2442	O	THR	206	14.057	78.457	42.730	1.00	24.79	B
ATOM	2443	N	GLU	207	13.713	80.626	43.274	1.00	29.47	B
ATOM	2444	H	GLU	207	13.932	81.567	43.109	1.00	0.00	B
ATOM	2445	CA	GLU	207	12.746	80.266	44.308	1.00	32.79	B
ATOM	2446	CB	GLU	207	12.209	81.492	45.089	1.00	38.54	B
ATOM	2447	CG	GLU	207	12.696	82.875	44.665	1.00	45.27	B
ATOM	2448	CD	GLU	207	11.738	84.002	45.104	1.00	52.80	B
ATOM	2449	OE1	GLU	207	11.106	84.632	44.220	1.00	49.46	B
ATOM	2450	OE2	GLU	207	11.618	84.260	46.330	1.00	48.25	B
ATOM	2451	C	GLU	207	11.582	79.567	43.623	1.00	30.36	B
ATOM	2452	O	GLU	207	11.141	78.499	44.052	1.00	29.14	B
ATOM	2453	N	GLU	208	11.108	80.172	42.538	1.00	30.06	B
ATOM	2454	H	GLU	208	11.527	81.005	42.237	1.00	0.00	B
ATOM	2455	CA	GLU	208	9.980	79.635	41.781	1.00	24.26	B
ATOM	2456	CB	GLU	208	9.588	80.606	40.680	1.00	25.42	B
ATOM	2457	CG	GLU	208	8.833	81.818	41.198	1.00	32.20	B
ATOM	2458	CD	GLU	208	8.830	82.953	40.203	1.00	37.03	B
ATOM	2459	OE1	GLU	208	7.763	83.243	39.623	1.00	39.29	B
ATOM	2460	OE2	GLU	208	9.900	83.551	40.000	1.00	39.74	B
ATOM	2461	C	GLU	208	10.223	78.265	41.174	1.00	20.07	B
ATOM	2462	O	GLU	208	9.308	77.465	41.049	1.00	24.58	B
ATOM	2463	N	VAL	209	11.459	78.000	40.783	1.00	17.97	B
ATOM	2464	H	VAL	209	12.154	78.681	40.891	1.00	0.00	B
ATOM	2465	CA	VAL	209	11.798	76.715	40.198	1.00	15.42	B
ATOM	2466	CB	VAL	209	13.158	76.797	39.466	1.00	18.29	B
ATOM	2467	CG1	VAL	209	13.810	75.418	39.380	1.00	13.02	B
ATOM	2468	CG2	VAL	209	12.946	77.399	38.087	1.00	13.44	B
ATOM	2469	C	VAL	209	11.860	75.669	41.308	1.00	16.08	B
ATOM	2470	O	VAL	209	11.460	74.521	41.110	1.00	17.96	B
ATOM	2471	N	LEU	210	12.345	76.074	42.480	1.00	23.26	B
ATOM	2472	H	LEU	210	12.643	77.004	42.575	1.00	0.00	B
ATOM	2473	CA	LEU	210	12.445	75.166	43.626	1.00	24.65	B
ATOM	2474	CB	LEU	210	13.202	75.824	44.777	1.00	19.16	B
ATOM	2475	CG	LEU	210	14.712	75.955	44.603	1.00	29.23	B
ATOM	2476	CD1	LEU	210	15.270	76.886	45.687	1.00	32.84	B
ATOM	2477	CD2	LEU	210	15.354	74.576	44.682	1.00	27.82	B
ATOM	2478	C	LEU	210	11.051	74.805	44.099	1.00	27.07	B
ATOM	2479	O	LEU	210	10.790	73.690	44.555	1.00	24.27	B
ATOM	2480	N	VAL	211	10.150	75.770	44.012	1.00	27.55	B
ATOM	2481	H	VAL	211	10.408	76.654	43.678	1.00	0.00	B
ATOM	2482	CA	VAL	211	8.787	75.518	44.414	1.00	24.35	B
ATOM	2483	CB	VAL	211	7.966	76.832	44.404	1.00	23.80	B
ATOM	2484	CG1	VAL	211	6.474	76.535	44.344	1.00	22.78	B
ATOM	2485	CG2	VAL	211	8.292	77.641	45.661	1.00	20.18	B
ATOM	2486	C	VAL	211	8.176	74.472	43.472	1.00	24.70	B
ATOM	2487	O	VAL	211	7.566	73.504	43.934	1.00	24.21	B
ATOM	2488	N	ALA	212	8.364	74.643	42.163	1.00	24.07	B
ATOM	2489	H	ALA	212	8.883	75.411	41.847	1.00	0.00	B
ATOM	2490	CA	ALA	212	7.806	73.695	41.183	1.00	23.91	B

ATOM	2491	CB	ALA	212	8.004	74.221	39.777	1.00	20.84	B
ATOM	2492	C	ALA	212	8.416	72.299	41.279	1.00	23.54	B
ATOM	2493	O	ALA	212	7.709	71.280	41.195	1.00	19.74	B
ATOM	2494	N	ALA	213	9.736	72.270	41.433	1.00	22.17	B
ATOM	2495	H	ALA	213	10.220	73.119	41.495	1.00	0.00	B
ATOM	2496	CA	ALA	213	10.484	71.032	41.516	1.00	20.06	B
ATOM	2497	CB	ALA	213	11.966	71.332	41.523	1.00	23.28	B
ATOM	2498	C	ALA	213	10.096	70.259	42.763	1.00	24.35	B
ATOM	2499	O	ALA	213	10.032	69.034	42.748	1.00	24.95	B
ATOM	2500	N	ASN	214	9.819	70.969	43.844	1.00	24.25	B
ATOM	2501	H	ASN	214	9.875	71.949	43.812	1.00	0.00	B
ATOM	2502	CA	ASN	214	9.434	70.304	45.086	1.00	24.82	B
ATOM	2503	CB	ASN	214	9.604	71.247	46.273	1.00	26.46	B
ATOM	2504	CG	ASN	214	10.981	71.151	46.882	1.00	28.78	B
ATOM	2505	OD1	ASN	214	11.870	71.958	46.578	1.00	23.63	B
ATOM	2506	ND2	ASN	214	11.179	70.153	47.739	1.00	25.69	B
ATOM	2507	HD21	ASN	214	10.444	69.533	47.941	1.00	0.00	B
ATOM	2508	HD22	ASN	214	12.063	70.070	48.145	1.00	0.00	B
ATOM	2509	C	ASN	214	8.013	69.755	45.069	1.00	24.64	B
ATOM	2510	O	ASN	214	7.606	69.021	45.974	1.00	18.78	B
ATOM	2511	N	LYS	215	7.256	70.103	44.039	1.00	23.65	B
ATOM	2512	H	LYS	215	7.617	70.696	43.345	1.00	0.00	B
ATOM	2513	CA	LYS	215	5.901	69.609	43.933	1.00	26.33	B
ATOM	2514	CB	LYS	215	4.961	70.746	43.526	1.00	22.52	B
ATOM	2515	CG	LYS	215	4.196	71.337	44.708	1.00	28.33	B
ATOM	2516	CD	LYS	215	3.432	72.606	44.316	1.00	32.87	B
ATOM	2517	CE	LYS	215	1.978	72.307	43.951	1.00	30.67	B
ATOM	2518	NZ	LYS	215	1.649	72.846	42.601	1.00	35.42	B
ATOM	2519	HZ1	LYS	215	2.271	72.406	41.892	1.00	0.00	B
ATOM	2520	HZ2	LYS	215	1.791	73.875	42.596	1.00	0.00	B
ATOM	2521	HZ3	LYS	215	0.658	72.630	42.375	1.00	0.00	B
ATOM	2522	C	LYS	215	5.760	68.434	42.960	1.00	22.45	B
ATOM	2523	O	LYS	215	4.662	67.926	42.764	1.00	30.36	B
ATOM	2524	N	ILE	216	6.864	67.976	42.375	1.00	16.84	B
ATOM	2525	H	ILE	216	7.734	68.373	42.593	1.00	0.00	B
ATOM	2526	CA	ILE	216	6.781	66.884	41.415	1.00	12.02	B
ATOM	2527	CB	ILE	216	8.023	66.856	40.498	1.00	14.58	B
ATOM	2528	CG2	ILE	216	8.050	65.566	39.671	1.00	19.30	B
ATOM	2529	CG1	ILE	216	8.007	68.084	39.574	1.00	13.98	B
ATOM	2530	CD1	ILE	216	9.345	68.390	38.904	1.00	13.34	B
ATOM	2531	C	ILE	216	6.586	65.514	42.061	1.00	12.93	B
ATOM	2532	O	ILE	216	7.311	65.135	42.980	1.00	15.03	B
ATOM	2533	N	GLY	217	5.581	64.785	41.580	1.00	17.89	B
ATOM	2534	H	GLY	217	5.022	65.150	40.868	1.00	0.00	B
ATOM	2535	CA	GLY	217	5.304	63.452	42.103	1.00	17.34	B
ATOM	2536	C	GLY	217	5.749	62.385	41.112	1.00	14.75	B
ATOM	2537	O	GLY	217	5.675	62.588	39.898	1.00	15.21	B
ATOM	2538	N	ARG	218	6.207	61.248	41.631	1.00	14.09	B
ATOM	2539	H	ARG	218	6.226	61.146	42.604	1.00	0.00	B
ATOM	2540	CA	ARG	218	6.683	60.152	40.797	1.00	17.47	B
ATOM	2541	CB	ARG	218	7.195	59.023	41.707	1.00	21.57	B
ATOM	2542	CG	ARG	218	6.442	57.725	41.637	1.00	25.79	B
ATOM	2543	CD	ARG	218	7.384	56.563	41.388	1.00	22.17	B
ATOM	2544	NE	ARG	218	7.509	55.752	42.588	1.00	16.26	B
ATOM	2545	HE	ARG	218	6.793	55.112	42.782	1.00	0.00	B
ATOM	2546	CZ	ARG	218	8.531	55.814	43.431	1.00	16.32	B
ATOM	2547	NH1	ARG	218	9.521	56.644	43.210	1.00	28.95	B
ATOM	2548	HH11	ARG	218	9.511	57.229	42.399	1.00	0.00	B
ATOM	2549	HH12	ARG	218	10.287	56.689	43.849	1.00	0.00	B
ATOM	2550	NH2	ARG	218	8.546	55.054	44.512	1.00	33.70	B
ATOM	2551	HH21	ARG	218	7.789	54.425	44.693	1.00	0.00	B
ATOM	2552	HH22	ARG	218	9.316	55.104	45.146	1.00	0.00	B
ATOM	2553	C	ARG	218	5.533	59.701	39.912	1.00	14.35	B
ATOM	2554	O	ARG	218	4.524	59.251	40.405	1.00	19.15	B
ATOM	2555	N	GLN	219	5.670	59.815	38.597	1.00	17.48	B
ATOM	2556	H	GLN	219	6.506	60.148	38.210	1.00	0.00	B
ATOM	2557	CA	GLN	219	4.552	59.438	37.749	1.00	26.72	B
ATOM	2558	CB	GLN	219	4.664	60.107	36.363	1.00	23.72	B
ATOM	2559	CG	GLN	219	5.223	59.280	35.221	1.00	25.69	B
ATOM	2560	CD	GLN	219	5.649	60.171	34.056	1.00	33.29	B
ATOM	2561	OE1	GLN	219	5.982	61.346	34.257	1.00	26.70	B
ATOM	2562	NE2	GLN	219	5.634	59.627	32.832	1.00	18.76	B
ATOM	2563	HE21	GLN	219	5.360	58.692	32.720	1.00	0.00	B

ATOM	2564	HE22	GLN	219	5.906	60.191	32.081	1.00	0.00	B
ATOM	2565	C	GLN	219	4.344	57.935	37.650	1.00	26.26	B
ATOM	2566	O	GLN	219	3.210	57.475	37.527	1.00	30.40	B
ATOM	2567	N	GLY	220	5.419	57.166	37.745	1.00	26.30	B
ATOM	2568	H	GLY	220	6.305	57.568	37.863	1.00	0.00	B
ATOM	2569	CA	GLY	220	5.270	55.728	37.672	1.00	30.10	B
ATOM	2570	C	GLY	220	5.364	55.123	36.282	1.00	29.97	B
ATOM	2571	O	GLY	220	5.002	55.740	35.277	1.00	33.59	B
ATOM	2572	N	GLY	221	5.849	53.889	36.244	1.00	35.79	B
ATOM	2573	H	GLY	221	6.109	53.453	37.082	1.00	0.00	B
ATOM	2574	CA	GLY	221	6.004	53.171	34.998	1.00	39.72	B
ATOM	2575	C	GLY	221	6.406	51.736	35.283	1.00	40.82	B
ATOM	2576	O	GLY	221	7.085	51.463	36.277	1.00	41.96	B
ATOM	2577	N	LEU	222	5.974	50.822	34.422	1.00	37.83	B
ATOM	2578	H	LEU	222	5.424	51.109	33.665	1.00	0.00	B
ATOM	2579	CA	LEU	222	6.288	49.402	34.564	1.00	41.13	B
ATOM	2580	CB	LEU	222	5.102	48.543	34.103	1.00	42.69	B
ATOM	2581	CG	LEU	222	4.467	47.593	35.126	1.00	48.06	B
ATOM	2582	CD1	LEU	222	4.063	48.361	36.380	1.00	47.26	B
ATOM	2583	CD2	LEU	222	3.259	46.917	34.509	1.00	44.76	B
ATOM	2584	C	LEU	222	7.506	49.093	33.707	1.00	39.93	B
ATOM	2585	O	LEU	222	8.193	48.099	33.931	1.00	42.67	B
ATOM	2586	N	GLN	223	7.755	49.954	32.723	1.00	35.86	B
ATOM	2587	H	GLN	223	7.145	50.711	32.601	1.00	0.00	B
ATOM	2588	CA	GLN	223	8.893	49.825	31.815	1.00	35.26	B
ATOM	2589	CB	GLN	223	8.419	49.479	30.396	1.00	37.16	B
ATOM	2590	CG	GLN	223	6.995	48.952	30.328	0.01	41.99	B
ATOM	2591	CD	GLN	223	6.839	47.821	29.332	0.01	44.07	B
ATOM	2592	OE1	GLN	223	7.368	46.726	29.528	0.01	45.41	B
ATOM	2593	NE2	GLN	223	6.109	48.080	28.253	0.01	44.90	B
ATOM	2594	HE21	GLN	223	5.707	48.966	28.138	1.00	0.00	B
ATOM	2595	HE22	GLN	223	5.997	47.364	27.601	1.00	0.00	B
ATOM	2596	C	GLN	223	9.642	51.160	31.799	1.00	32.91	B
ATOM	2597	O	GLN	223	9.032	52.218	31.641	1.00	24.75	B
ATOM	2598	N	THR	224	10.961	51.096	31.969	1.00	30.99	B
ATOM	2599	H	THR	224	11.378	50.218	32.084	1.00	0.00	B
ATOM	2600	CA	THR	224	11.814	52.283	31.989	1.00	25.14	B
ATOM	2601	CB	THR	224	13.016	52.047	32.891	1.00	22.33	B
ATOM	2602	OG1	THR	224	12.548	51.636	34.177	1.00	22.14	B
ATOM	2603	HG1	THR	224	12.042	50.826	34.091	1.00	0.00	B
ATOM	2604	CG2	THR	224	13.850	53.315	33.025	1.00	16.21	B
ATOM	2605	C	THR	224	12.295	52.644	30.590	1.00	24.48	B
ATOM	2606	O	THR	224	13.197	52.010	30.042	1.00	22.45	B
ATOM	2607	N	MET	225	11.695	53.688	30.027	1.00	23.62	B
ATOM	2608	H	MET	225	11.019	54.182	30.535	1.00	0.00	B
ATOM	2609	CA	MET	225	12.015	54.118	28.673	1.00	21.06	B
ATOM	2610	CB	MET	225	10.708	54.410	27.944	1.00	20.26	B
ATOM	2611	CG	MET	225	9.719	53.257	28.063	1.00	24.98	B
ATOM	2612	SD	MET	225	10.320	51.746	27.262	1.00	25.64	B
ATOM	2613	CE	MET	225	10.098	52.166	25.621	1.00	19.80	B
ATOM	2614	C	MET	225	12.943	55.327	28.629	1.00	20.97	B
ATOM	2615	O	MET	225	12.562	56.408	28.185	1.00	23.42	B
ATOM	2616	N	THR	226	14.177	55.119	29.062	1.00	22.97	B
ATOM	2617	H	THR	226	14.433	54.221	29.359	1.00	0.00	B
ATOM	2618	CA	THR	226	15.163	56.187	29.111	1.00	18.05	B
ATOM	2619	CB	THR	226	16.487	55.667	29.700	1.00	20.16	B
ATOM	2620	OG1	THR	226	16.212	54.950	30.912	1.00	13.45	B
ATOM	2621	HG1	THR	226	15.789	55.535	31.542	1.00	0.00	B
ATOM	2622	CG2	THR	226	17.418	56.826	30.012	1.00	15.25	B
ATOM	2623	C	THR	226	15.411	56.836	27.767	1.00	17.23	B
ATOM	2624	O	THR	226	15.468	58.059	27.681	1.00	15.63	B
ATOM	2625	N	ALA	227	15.546	56.028	26.717	1.00	13.67	B
ATOM	2626	H	ALA	227	15.502	55.057	26.849	1.00	0.00	B
ATOM	2627	CA	ALA	227	15.768	56.558	25.381	1.00	14.13	B
ATOM	2628	CB	ALA	227	16.028	55.431	24.382	1.00	5.26	B
ATOM	2629	C	ALA	227	14.625	57.430	24.879	1.00	20.64	B
ATOM	2630	O	ALA	227	14.862	58.332	24.067	1.00	30.73	B
ATOM	2631	N	LEU	228	13.396	57.142	25.323	1.00	24.49	B
ATOM	2632	H	LEU	228	13.283	56.379	25.927	1.00	0.00	B
ATOM	2633	CA	LEU	228	12.208	57.920	24.948	1.00	20.92	B
ATOM	2634	CB	LEU	228	10.918	57.301	25.507	1.00	28.56	B
ATOM	2635	CG	LEU	228	9.604	57.195	24.708	1.00	36.02	B
ATOM	2636	CD1	LEU	228	8.424	57.532	25.623	1.00	32.15	B

ATOM	2637	CD2	LEU	228	9.615	58.114	23.504	1.00	38.46	B
ATOM	2638	C	LEU	228	12.349	59.295	25.577	1.00	20.10	B
ATOM	2639	O	LEU	228	12.252	60.307	24.894	1.00	21.88	B
ATOM	2640	N	GLY	229	12.551	59.309	26.895	1.00	17.67	B
ATOM	2641	H	GLY	229	12.605	58.462	27.383	1.00	0.00	B
ATOM	2642	CA	GLY	229	12.692	60.562	27.618	1.00	17.97	B
ATOM	2643	C	GLY	229	13.757	61.507	27.070	1.00	16.62	B
ATOM	2644	O	GLY	229	13.513	62.691	26.912	1.00	16.95	B
ATOM	2645	N	THR	230	14.934	60.964	26.780	1.00	14.32	B
ATOM	2646	H	THR	230	15.056	60.004	26.924	1.00	0.00	B
ATOM	2647	CA	THR	230	16.052	61.731	26.255	1.00	13.65	B
ATOM	2648	CB	THR	230	17.311	60.832	26.166	1.00	13.38	B
ATOM	2649	OG1	THR	230	17.904	60.705	27.472	1.00	24.82	B
ATOM	2650	HG1	THR	230	18.154	61.573	27.796	1.00	0.00	B
ATOM	2651	CG2	THR	230	18.331	61.413	25.195	1.00	16.39	B
ATOM	2652	C	THR	230	15.722	62.276	24.865	1.00	16.56	B
ATOM	2653	O	THR	230	15.923	63.452	24.580	1.00	14.40	B
ATOM	2654	N	ASP	231	15.223	61.400	24.008	1.00	11.84	B
ATOM	2655	H	ASP	231	15.086	60.475	24.300	1.00	0.00	B
ATOM	2656	CA	ASP	231	14.874	61.768	22.658	1.00	20.60	B
ATOM	2657	CB	ASP	231	14.400	60.521	21.911	1.00	23.12	B
ATOM	2658	CG	ASP	231	14.401	60.703	20.421	1.00	23.62	B
ATOM	2659	OD1	ASP	231	15.451	61.103	19.881	1.00	26.06	B
ATOM	2660	OD2	ASP	231	13.363	60.450	19.788	1.00	19.93	B
ATOM	2661	C	ASP	231	13.772	62.832	22.663	1.00	21.87	B
ATOM	2662	O	ASP	231	13.800	63.799	21.898	1.00	20.06	B
ATOM	2663	N	THR	232	12.804	62.637	23.544	1.00	22.80	B
ATOM	2664	H	THR	232	12.854	61.855	24.132	1.00	0.00	B
ATOM	2665	CA	THR	232	11.670	63.537	23.681	1.00	22.51	B
ATOM	2666	CB	THR	232	10.622	62.891	24.609	1.00	16.89	B
ATOM	2667	OG1	THR	232	10.277	61.607	24.075	1.00	21.61	B
ATOM	2668	HG1	THR	232	11.061	61.055	24.031	1.00	0.00	B
ATOM	2669	CG2	THR	232	9.372	63.733	24.706	1.00	20.59	B
ATOM	2670	C	THR	232	12.115	64.903	24.201	1.00	25.12	B
ATOM	2671	O	THR	232	11.601	65.952	23.782	1.00	25.24	B
ATOM	2672	N	ALA	233	13.091	64.882	25.098	1.00	21.55	B
ATOM	2673	H	ALA	233	13.457	64.019	25.383	1.00	0.00	B
ATOM	2674	CA	ALA	233	13.635	66.099	25.674	1.00	17.44	B
ATOM	2675	CB	ALA	233	14.498	65.746	26.865	1.00	17.88	B
ATOM	2676	C	ALA	233	14.453	66.855	24.624	1.00	19.30	B
ATOM	2677	O	ALA	233	14.394	68.075	24.533	1.00	18.02	B
ATOM	2678	N	ARG	234	15.197	66.115	23.815	1.00	17.81	B
ATOM	2679	H	ARG	234	15.196	65.141	23.918	1.00	0.00	B
ATOM	2680	CA	ARG	234	16.008	66.723	22.774	1.00	23.98	B
ATOM	2681	CB	ARG	234	16.857	65.647	22.087	1.00	25.23	B
ATOM	2682	CG	ARG	234	17.603	66.121	20.851	1.00	28.43	B
ATOM	2683	CD	ARG	234	18.028	64.952	19.994	1.00	25.37	B
ATOM	2684	NE	ARG	234	17.098	64.763	18.887	1.00	35.93	B
ATOM	2685	HE	ARG	234	16.794	65.558	18.403	1.00	0.00	B
ATOM	2686	CZ	ARG	234	16.642	63.584	18.494	1.00	33.70	B
ATOM	2687	NH1	ARG	234	17.036	62.484	19.120	1.00	42.49	B
ATOM	2688	HH11	ARG	234	17.678	62.545	19.883	1.00	0.00	B
ATOM	2689	HH12	ARG	234	16.693	61.592	18.824	1.00	0.00	B
ATOM	2690	NH2	ARG	234	15.786	63.507	17.488	1.00	34.51	B
ATOM	2691	HH21	ARG	234	15.485	64.341	17.023	1.00	0.00	B
ATOM	2692	HH22	ARG	234	15.439	62.618	17.192	1.00	0.00	B
ATOM	2693	C	ARG	234	15.071	67.341	21.747	1.00	23.74	B
ATOM	2694	O	ARG	234	15.212	68.500	21.327	1.00	19.58	B
ATOM	2695	N	LYS	235	14.099	66.535	21.360	1.00	22.00	B
ATOM	2696	H	LYS	235	14.031	65.650	21.771	1.00	0.00	B
ATOM	2697	CA	LYS	235	13.136	66.915	20.349	1.00	23.75	B
ATOM	2698	CB	LYS	235	12.365	65.674	19.907	1.00	27.18	B
ATOM	2699	CG	LYS	235	12.541	65.347	18.434	1.00	39.17	B
ATOM	2700	CD	LYS	235	12.592	63.848	18.206	1.00	40.05	B
ATOM	2701	CE	LYS	235	11.203	63.255	18.179	1.00	37.98	B
ATOM	2702	NZ	LYS	235	11.172	62.081	17.280	1.00	36.28	B
ATOM	2703	HZ1	LYS	235	11.846	61.365	17.624	1.00	0.00	B
ATOM	2704	HZ2	LYS	235	11.440	62.374	16.319	1.00	0.00	B
ATOM	2705	HZ3	LYS	235	10.215	61.679	17.267	1.00	0.00	B
ATOM	2706	C	LYS	235	12.159	67.992	20.776	1.00	14.66	B
ATOM	2707	O	LYS	235	11.854	68.867	20.003	1.00	15.35	B
ATOM	2708	N	GLU	236	11.698	67.938	22.017	1.00	19.61	B
ATOM	2709	H	GLU	236	12.029	67.243	22.621	1.00	0.00	B

ATOM	2710	CA	GLU	236	10.714	68.893	22.491	1.00	19.56	B
ATOM	2711	CB	GLU	236	9.467	68.131	22.980	1.00	17.41	B
ATOM	2712	CG	GLU	236	8.705	67.442	21.848	1.00	12.51	B
ATOM	2713	CD	GLU	236	7.734	66.365	22.326	1.00	20.23	B
ATOM	2714	OE1	GLU	236	7.147	66.493	23.416	1.00	16.25	B
ATOM	2715	OE2	GLU	236	7.553	65.382	21.594	1.00	32.75	B
ATOM	2716	C	GLU	236	11.134	69.905	23.552	1.00	19.85	B
ATOM	2717	O	GLU	236	10.740	71.074	23.477	1.00	22.57	B
ATOM	2718	N	ALA	237	11.923	69.477	24.530	1.00	13.82	B
ATOM	2719	H	ALA	237	12.243	68.552	24.528	1.00	0.00	B
ATOM	2720	CA	ALA	237	12.320	70.380	25.609	1.00	15.91	B
ATOM	2721	CB	ALA	237	13.031	69.599	26.715	1.00	12.47	B
ATOM	2722	C	ALA	237	13.183	71.568	25.185	1.00	18.22	B
ATOM	2723	O	ALA	237	13.067	72.647	25.754	1.00	20.95	B
ATOM	2724	N	PHE	238	14.050	71.372	24.202	1.00	20.05	B
ATOM	2725	H	PHE	238	14.094	70.495	23.767	1.00	0.00	B
ATOM	2726	CA	PHE	238	14.938	72.443	23.757	1.00	25.75	B
ATOM	2727	CB	PHE	238	16.286	71.864	23.411	1.00	21.10	B
ATOM	2728	CG	PHE	238	17.058	71.430	24.607	1.00	20.59	B
ATOM	2729	CD1	PHE	238	17.153	70.081	24.926	1.00	10.70	B
ATOM	2730	CD2	PHE	238	17.690	72.378	25.425	1.00	17.21	B
ATOM	2731	CE1	PHE	238	17.865	69.668	26.043	1.00	6.53	B
ATOM	2732	CE2	PHE	238	18.407	71.981	26.548	1.00	9.67	B
ATOM	2733	CZ	PHE	238	18.498	70.623	26.860	1.00	14.30	B
ATOM	2734	C	PHE	238	14.364	73.171	22.570	1.00	32.55	B
ATOM	2735	O	PHE	238	15.050	73.472	21.591	1.00	34.64	B
ATOM	2736	N	THR	239	13.080	73.446	22.682	1.00	33.09	B
ATOM	2737	H	THR	239	12.608	73.176	23.499	1.00	0.00	B
ATOM	2738	CA	THR	239	12.344	74.125	21.651	1.00	37.89	B
ATOM	2739	CB	THR	239	10.911	73.562	21.597	1.00	34.14	B
ATOM	2740	OG1	THR	239	10.907	72.378	20.797	1.00	44.61	B
ATOM	2741	HG1	THR	239	10.019	72.020	20.758	1.00	0.00	B
ATOM	2742	CG2	THR	239	9.953	74.558	21.010	1.00	42.52	B
ATOM	2743	C	THR	239	12.329	75.606	21.986	1.00	38.96	B
ATOM	2744	O	THR	239	12.421	75.989	23.156	1.00	40.40	B
ATOM	2745	N	GLU	240	12.229	76.438	20.962	1.00	36.75	B
ATOM	2746	H	GLU	240	12.181	76.087	20.049	1.00	0.00	B
ATOM	2747	CA	GLU	240	12.191	77.867	21.185	1.00	42.75	B
ATOM	2748	CB	GLU	240	12.344	78.604	19.855	1.00	50.61	B
ATOM	2749	CG	GLU	240	11.038	78.872	19.148	1.00	62.98	B
ATOM	2750	CD	GLU	240	10.313	80.068	19.724	1.00	67.81	B
ATOM	2751	OE1	GLU	240	10.925	81.156	19.774	1.00	70.98	B
ATOM	2752	OE2	GLU	240	9.140	79.916	20.131	1.00	69.99	B
ATOM	2753	C	GLU	240	10.843	78.178	21.843	1.00	40.19	B
ATOM	2754	O	GLU	240	10.751	79.041	22.707	1.00	33.66	B
ATOM	2755	N	ALA	241	9.804	77.458	21.423	1.00	33.98	B
ATOM	2756	H	ALA	241	9.936	76.796	20.714	1.00	0.00	B
ATOM	2757	CA	ALA	241	8.471	77.636	21.986	1.00	29.60	B
ATOM	2758	CB	ALA	241	7.492	76.687	21.316	1.00	37.19	B
ATOM	2759	C	ALA	241	8.499	77.375	23.491	1.00	29.07	B
ATOM	2760	O	ALA	241	7.801	78.047	24.251	1.00	32.90	B
ATOM	2761	N	ARG	242	9.312	76.406	23.916	1.00	25.07	B
ATOM	2762	H	ARG	242	9.845	75.913	23.257	1.00	0.00	B
ATOM	2763	CA	ARG	242	9.429	76.057	25.332	1.00	21.30	B
ATOM	2764	CB	ARG	242	9.644	74.551	25.495	1.00	21.86	B
ATOM	2765	CG	ARG	242	8.486	73.680	24.980	1.00	18.40	B
ATOM	2766	CD	ARG	242	8.520	72.317	25.663	1.00	23.54	B
ATOM	2767	NE	ARG	242	7.674	71.334	25.001	1.00	27.29	B
ATOM	2768	HE	ARG	242	7.958	70.990	24.131	1.00	0.00	B
ATOM	2769	CZ	ARG	242	6.536	70.870	25.509	1.00	21.77	B
ATOM	2770	NH1	ARG	242	6.106	71.302	26.686	1.00	28.61	B
ATOM	2771	HH11	ARG	242	6.637	71.979	27.196	1.00	0.00	B
ATOM	2772	HH12	ARG	242	5.249	70.952	27.064	1.00	0.00	B
ATOM	2773	NH2	ARG	242	5.842	69.967	24.851	1.00	21.18	B
ATOM	2774	HH21	ARG	242	6.171	69.625	23.969	1.00	0.00	B
ATOM	2775	HH22	ARG	242	4.986	69.618	25.232	1.00	0.00	B
ATOM	2776	C	ARG	242	10.538	76.806	26.071	1.00	17.43	B
ATOM	2777	O	ARG	242	10.884	76.462	27.206	1.00	14.43	B
ATOM	2778	N	GLY	243	11.127	77.800	25.419	1.00	15.32	B
ATOM	2779	H	GLY	243	10.878	78.002	24.495	1.00	0.00	B
ATOM	2780	CA	GLY	243	12.146	78.595	26.096	1.00	16.02	B
ATOM	2781	C	GLY	243	13.628	78.505	25.786	1.00	10.54	B
ATOM	2782	O	GLY	243	14.406	79.182	26.444	1.00	20.03	B

ATOM	2783	N	ALA	244	14.038	77.716	24.801	1.00	10.60	B
ATOM	2784	H	ALA	244	13.378	77.200	24.293	1.00	0.00	B
ATOM	2785	CA	ALA	244	15.453	77.610	24.476	1.00	10.63	B
ATOM	2786	CB	ALA	244	15.692	76.439	23.533	1.00	12.74	B
ATOM	2787	C	ALA	244	15.916	78.907	23.828	1.00	19.09	B
ATOM	2788	O	ALA	244	15.394	79.329	22.800	1.00	22.97	B
ATOM	2789	N	ARG	245	16.911	79.540	24.433	1.00	21.88	B
ATOM	2790	H	ARG	245	17.308	79.140	25.235	1.00	0.00	B
ATOM	2791	CA	ARG	245	17.429	80.809	23.942	1.00	16.43	B
ATOM	2792	CB	ARG	245	18.037	81.552	25.122	1.00	16.53	B
ATOM	2793	CG	ARG	245	17.062	81.593	26.288	1.00	18.89	B
ATOM	2794	CD	ARG	245	17.668	82.162	27.546	1.00	20.31	B
ATOM	2795	NE	ARG	245	18.429	81.148	28.265	1.00	12.05	B
ATOM	2796	HE	ARG	245	18.290	80.209	28.024	1.00	0.00	B
ATOM	2797	CZ	ARG	245	19.290	81.427	29.230	1.00	16.66	B
ATOM	2798	NH1	ARG	245	19.494	82.692	29.589	1.00	11.02	B
ATOM	2799	HH11	ARG	245	18.992	83.428	29.138	1.00	0.00	B
ATOM	2800	HH12	ARG	245	20.147	82.907	30.317	1.00	0.00	B
ATOM	2801	NH2	ARG	245	19.949	80.444	29.830	1.00	17.95	B
ATOM	2802	HH21	ARG	245	19.789	79.495	29.554	1.00	0.00	B
ATOM	2803	HH22	ARG	245	20.604	80.649	30.554	1.00	0.00	B
ATOM	2804	C	ARG	245	18.411	80.701	22.784	1.00	13.58	B
ATOM	2805	O	ARG	245	19.106	79.699	22.632	1.00	14.35	B
ATOM	2806	N	ARG	246	18.450	81.739	21.952	1.00	16.40	B
ATOM	2807	H	ARG	246	17.864	82.504	22.119	1.00	0.00	B
ATOM	2808	CA	ARG	246	19.341	81.766	20.794	1.00	16.73	B
ATOM	2809	CB	ARG	246	19.116	83.052	19.978	1.00	20.99	B
ATOM	2810	CG	ARG	246	19.775	83.037	18.582	1.00	27.27	B
ATOM	2811	CD	ARG	246	19.881	81.606	18.080	1.00	29.21	B
ATOM	2812	NE	ARG	246	20.716	81.432	16.898	1.00	40.75	B
ATOM	2813	HE	ARG	246	21.467	80.808	16.959	1.00	0.00	B
ATOM	2814	CZ	ARG	246	20.516	82.047	15.737	1.00	40.49	B
ATOM	2815	NH1	ARG	246	19.502	82.893	15.590	1.00	44.89	B
ATOM	2816	HH11	ARG	246	18.867	83.049	16.346	1.00	0.00	B
ATOM	2817	HH12	ARG	246	19.361	83.355	14.715	1.00	0.00	B
ATOM	2818	NH2	ARG	246	21.323	81.797	14.715	1.00	40.11	B
ATOM	2819	HH21	ARG	246	22.065	81.130	14.816	1.00	0.00	B
ATOM	2820	HH22	ARG	246	21.185	82.260	13.841	1.00	0.00	B
ATOM	2821	C	ARG	246	20.830	81.662	21.175	1.00	19.16	B
ATOM	2822	O	ARG	246	21.347	82.479	21.929	1.00	19.43	B
ATOM	2823	N	GLY	247	21.505	80.652	20.651	1.00	15.61	B
ATOM	2824	H	GLY	247	21.040	80.009	20.075	1.00	0.00	B
ATOM	2825	CA	GLY	247	22.920	80.479	20.917	1.00	19.07	B
ATOM	2826	C	GLY	247	23.301	80.022	22.315	1.00	19.74	B
ATOM	2827	O	GLY	247	24.479	79.869	22.618	1.00	24.75	B
ATOM	2828	N	VAL	248	22.320	79.793	23.170	1.00	18.96	B
ATOM	2829	H	VAL	248	21.390	79.916	22.891	1.00	0.00	B
ATOM	2830	CA	VAL	248	22.619	79.361	24.528	1.00	16.15	B
ATOM	2831	CB	VAL	248	21.466	79.725	25.475	1.00	11.70	B
ATOM	2832	CG1	VAL	248	21.742	79.172	26.871	1.00	8.03	B
ATOM	2833	CG2	VAL	248	21.285	81.254	25.517	1.00	12.88	B
ATOM	2834	C	VAL	248	22.851	77.852	24.542	1.00	19.75	B
ATOM	2835	O	VAL	248	22.051	77.104	24.008	1.00	20.58	B
ATOM	2836	N	LYS	249	23.946	77.410	25.153	1.00	21.97	B
ATOM	2837	H	LYS	249	24.551	78.054	25.574	1.00	0.00	B
ATOM	2838	CA	LYS	249	24.269	75.983	25.204	1.00	24.74	B
ATOM	2839	CB	LYS	249	25.668	75.769	25.795	1.00	28.79	B
ATOM	2840	CG	LYS	249	26.782	75.746	24.731	1.00	39.64	B
ATOM	2841	CD	LYS	249	26.332	76.365	23.395	1.00	40.06	B
ATOM	2842	CE	LYS	249	27.485	76.507	22.393	1.00	46.49	B
ATOM	2843	NZ	LYS	249	28.289	77.759	22.567	1.00	42.34	B
ATOM	2844	HZ1	LYS	249	28.706	77.775	23.518	1.00	0.00	B
ATOM	2845	HZ2	LYS	249	27.672	78.587	22.444	1.00	0.00	B
ATOM	2846	HZ3	LYS	249	29.047	77.784	21.855	1.00	0.00	B
ATOM	2847	C	LYS	249	23.268	75.105	25.945	1.00	18.56	B
ATOM	2848	O	LYS	249	22.753	75.467	27.007	1.00	15.02	B
ATOM	2849	N	LYS	250	23.030	73.937	25.359	1.00	19.31	B
ATOM	2850	H	LYS	250	23.514	73.734	24.531	1.00	0.00	B
ATOM	2851	CA	LYS	250	22.101	72.943	25.864	1.00	21.51	B
ATOM	2852	CB	LYS	250	21.440	72.228	24.684	1.00	21.98	B
ATOM	2853	CG	LYS	250	20.819	73.146	23.641	1.00	24.29	B
ATOM	2854	CD	LYS	250	20.380	72.344	22.404	1.00	20.75	B
ATOM	2855	CE	LYS	250	19.318	73.084	21.606	1.00	30.12	B

ATOM	2856	NZ	LYS	250	19.629	73.074	20.143	1.00	33.42	B
ATOM	2857	HZ1	LYS	250	19.675	72.092	19.805	1.00	0.00	B
ATOM	2858	HZ2	LYS	250	20.546	73.539	19.983	1.00	0.00	B
ATOM	2859	HZ3	LYS	250	18.887	73.586	19.627	1.00	0.00	B
ATOM	2860	C	LYS	250	22.735	71.894	26.776	1.00	23.57	B
ATOM	2861	O	LYS	250	23.707	71.221	26.394	1.00	20.92	B
ATOM	2862	N	VAL	251	22.198	71.756	27.986	1.00	17.38	B
ATOM	2863	H	VAL	251	21.459	72.339	28.260	1.00	0.00	B
ATOM	2864	CA	VAL	251	22.708	70.748	28.899	1.00	17.18	B
ATOM	2865	CB	VAL	251	23.364	71.338	30.175	1.00	11.43	B
ATOM	2866	CG1	VAL	251	23.853	70.213	31.024	1.00	6.20	B
ATOM	2867	CG2	VAL	251	24.542	72.269	29.823	1.00	18.54	B
ATOM	2868	C	VAL	251	21.573	69.834	29.354	1.00	20.95	B
ATOM	2869	O	VAL	251	20.496	70.283	29.712	1.00	17.19	B
ATOM	2870	N	MET	252	21.831	68.537	29.332	1.00	17.99	B
ATOM	2871	H	MET	252	22.706	68.228	29.021	1.00	0.00	B
ATOM	2872	CA	MET	252	20.851	67.573	29.762	1.00	18.29	B
ATOM	2873	CB	MET	252	20.513	66.658	28.570	1.00	17.87	B
ATOM	2874	CG	MET	252	19.355	65.715	28.776	1.00	17.10	B
ATOM	2875	SD	MET	252	19.057	64.546	27.405	1.00	35.69	B
ATOM	2876	CE	MET	252	18.612	65.592	26.112	1.00	19.60	B
ATOM	2877	C	MET	252	21.451	66.778	30.932	1.00	15.72	B
ATOM	2878	O	MET	252	22.568	66.280	30.827	1.00	19.38	B
ATOM	2879	N	VAL	253	20.731	66.696	32.048	1.00	18.09	B
ATOM	2880	H	VAL	253	19.881	67.176	32.096	1.00	0.00	B
ATOM	2881	CA	VAL	253	21.165	65.916	33.208	1.00	17.72	B
ATOM	2882	CB	VAL	253	21.201	66.788	34.496	1.00	16.44	B
ATOM	2883	CG1	VAL	253	22.061	68.051	34.263	1.00	9.88	B
ATOM	2884	CG2	VAL	253	19.802	67.226	34.861	1.00	28.03	B
ATOM	2885	C	VAL	253	20.151	64.756	33.379	1.00	20.14	B
ATOM	2886	O	VAL	253	18.974	64.981	33.648	1.00	18.38	B
ATOM	2887	N	ILE	254	20.607	63.517	33.226	1.00	24.01	B
ATOM	2888	H	ILE	254	21.557	63.374	33.037	1.00	0.00	B
ATOM	2889	CA	ILE	254	19.715	62.360	33.335	1.00	20.30	B
ATOM	2890	CB	ILE	254	19.903	61.386	32.137	1.00	24.38	B
ATOM	2891	CG2	ILE	254	18.849	60.290	32.183	1.00	21.87	B
ATOM	2892	CG1	ILE	254	19.784	62.147	30.816	1.00	20.74	B
ATOM	2893	CD1	ILE	254	21.107	62.500	30.176	1.00	26.33	B
ATOM	2894	C	ILE	254	19.911	61.596	34.635	1.00	21.12	B
ATOM	2895	O	ILE	254	21.031	61.215	34.976	1.00	18.90	B
ATOM	2896	N	VAL	255	18.804	61.377	35.348	1.00	16.92	B
ATOM	2897	H	VAL	255	17.951	61.700	34.986	1.00	0.00	B
ATOM	2898	CA	VAL	255	18.796	60.692	36.629	1.00	16.15	B
ATOM	2899	CB	VAL	255	18.178	61.580	37.725	1.00	18.84	B
ATOM	2900	CG1	VAL	255	18.215	60.856	39.071	1.00	10.30	B
ATOM	2901	CG2	VAL	255	18.931	62.925	37.796	1.00	16.06	B
ATOM	2902	C	VAL	255	17.970	59.434	36.484	1.00	13.71	B
ATOM	2903	O	VAL	255	16.799	59.480	36.109	1.00	16.40	B
ATOM	2904	N	THR	256	18.584	58.301	36.781	1.00	14.62	B
ATOM	2905	H	THR	256	19.507	58.326	37.105	1.00	0.00	B
ATOM	2906	CA	THR	256	17.906	57.022	36.634	1.00	15.00	B
ATOM	2907	CB	THR	256	17.950	56.564	35.161	1.00	17.78	B
ATOM	2908	OG1	THR	256	17.186	55.359	35.006	1.00	23.15	B
ATOM	2909	HG1	THR	256	16.277	55.527	35.259	1.00	0.00	B
ATOM	2910	CG2	THR	256	19.414	56.327	34.704	1.00	10.75	B
ATOM	2911	C	THR	256	18.542	55.954	37.523	1.00	16.31	B
ATOM	2912	O	THR	256	19.740	56.041	37.862	1.00	16.43	B
ATOM	2913	N	ASP	257	17.739	54.948	37.881	1.00	15.42	B
ATOM	2914	H	ASP	257	16.815	54.937	37.553	1.00	0.00	B
ATOM	2915	CA	ASP	257	18.198	53.872	38.745	1.00	15.12	B
ATOM	2916	CB	ASP	257	17.481	53.974	40.119	1.00	17.76	B
ATOM	2917	CG	ASP	257	16.155	53.241	40.153	1.00	16.63	B
ATOM	2918	OD1	ASP	257	15.782	52.706	41.219	1.00	16.55	B
ATOM	2919	OD2	ASP	257	15.492	53.197	39.107	1.00	18.63	B
ATOM	2920	C	ASP	257	18.067	52.456	38.158	1.00	15.10	B
ATOM	2921	O	ASP	257	17.872	51.478	38.892	1.00	17.29	B
ATOM	2922	N	GLY	258	18.177	52.337	36.839	1.00	9.50	B
ATOM	2923	H	GLY	258	18.302	53.127	36.277	1.00	0.00	B
ATOM	2924	CA	GLY	258	18.108	51.013	36.240	1.00	11.28	B
ATOM	2925	C	GLY	258	18.275	50.992	34.737	1.00	13.51	B
ATOM	2926	O	GLY	258	18.350	52.038	34.108	1.00	17.36	B
ATOM	2927	N	GLU	259	18.328	49.792	34.159	1.00	16.87	B
ATOM	2928	H	GLU	259	18.257	48.995	34.723	1.00	0.00	B

ATOM	2929	CA	GLU	259	18.488	49.628	32.718	1.00	20.62	B
ATOM	2930	CB	GLU	259	18.730	48.158	32.358	1.00	23.36	B
ATOM	2931	CG	GLU	259	20.115	47.652	32.667	1.00	32.72	B
ATOM	2932	CD	GLU	259	20.119	46.175	33.015	1.00	31.78	B
ATOM	2933	OE1	GLU	259	19.803	45.356	32.120	1.00	30.21	B
ATOM	2934	OE2	GLU	259	20.441	45.844	34.178	1.00	27.13	B
ATOM	2935	C	GLU	259	17.238	50.083	32.003	1.00	22.02	B
ATOM	2936	O	GLU	259	16.141	50.060	32.571	1.00	22.92	B
ATOM	2937	N	SER	260	17.383	50.452	30.736	1.00	17.73	B
ATOM	2938	H	SER	260	18.264	50.419	30.314	1.00	0.00	B
ATOM	2939	CA	SER	260	16.226	50.900	29.987	1.00	21.31	B
ATOM	2940	CB	SER	260	16.609	52.107	29.133	1.00	18.50	B
ATOM	2941	OG	SER	260	17.456	51.716	28.080	1.00	19.64	B
ATOM	2942	HG	SER	260	18.255	51.324	28.441	1.00	0.00	B
ATOM	2943	C	SER	260	15.619	49.794	29.109	1.00	16.77	B
ATOM	2944	O	SER	260	16.330	49.027	28.486	1.00	16.79	B
ATOM	2945	N	HIS	261	14.292	49.719	29.083	1.00	20.77	B
ATOM	2946	H	HIS	261	13.775	50.351	29.622	1.00	0.00	B
ATOM	2947	CA	HIS	261	13.581	48.730	28.280	1.00	26.28	B
ATOM	2948	CB	HIS	261	12.074	48.819	28.545	1.00	36.28	B
ATOM	2949	CG	HIS	261	11.565	47.849	29.564	1.00	47.66	B
ATOM	2950	CD2	HIS	261	10.832	46.717	29.426	1.00	49.49	B
ATOM	2951	ND1	HIS	261	11.764	48.015	30.919	1.00	51.66	B
ATOM	2952	HD1	HIS	261	12.252	48.757	31.331	1.00	0.00	B
ATOM	2953	CE1	HIS	261	11.170	47.034	31.575	1.00	50.93	B
ATOM	2954	NE2	HIS	261	10.599	46.231	30.693	1.00	52.42	B
ATOM	2955	HE2	HIS	261	10.085	45.430	30.904	1.00	0.00	B
ATOM	2956	C	HIS	261	13.836	49.169	26.854	1.00	23.53	B
ATOM	2957	O	HIS	261	13.634	48.437	25.895	1.00	23.83	B
ATOM	2958	N	TYR	262	14.292	50.405	26.767	1.00	22.41	B
ATOM	2959	H	TYR	262	14.447	50.886	27.607	1.00	0.00	B
ATOM	2960	CA	TYR	262	14.581	51.112	25.537	1.00	22.32	B
ATOM	2961	CB	TYR	262	14.348	52.594	25.795	1.00	29.85	B
ATOM	2962	CG	TYR	262	13.305	53.169	24.914	1.00	35.37	B
ATOM	2963	CD1	TYR	262	12.587	54.264	25.316	1.00	29.84	B
ATOM	2964	CE1	TYR	262	11.582	54.781	24.522	1.00	46.06	B
ATOM	2965	CD2	TYR	262	13.009	52.594	23.671	1.00	41.64	B
ATOM	2966	CE2	TYR	262	11.987	53.118	22.858	1.00	46.38	B
ATOM	2967	CZ	TYR	262	11.281	54.224	23.302	1.00	41.00	B
ATOM	2968	OH	TYR	262	10.252	54.782	22.570	1.00	44.86	B
ATOM	2969	HH	TYR	262	10.120	54.276	21.766	1.00	0.00	B
ATOM	2970	C	TYR	262	15.981	50.955	24.943	1.00	21.72	B
ATOM	2971	O	TYR	262	16.269	51.550	23.903	1.00	17.28	B
ATOM	2972	N	ASN	263	16.839	50.201	25.628	1.00	23.04	B
ATOM	2973	H	ASN	263	16.526	49.784	26.457	1.00	0.00	B
ATOM	2974	CA	ASN	263	18.222	49.950	25.220	1.00	24.13	B
ATOM	2975	CB	ASN	263	18.634	48.513	25.584	1.00	29.95	B
ATOM	2976	CG	ASN	263	18.971	48.335	27.058	1.00	36.99	B
ATOM	2977	OD1	ASN	263	18.731	49.210	27.886	1.00	41.66	B
ATOM	2978	ND2	ASN	263	19.528	47.181	27.384	1.00	40.94	B
ATOM	2979	HD21	ASN	263	19.702	46.507	26.693	1.00	0.00	B
ATOM	2980	HD22	ASN	263	19.752	47.038	28.326	1.00	0.00	B
ATOM	2981	C	ASN	263	18.543	50.136	23.736	1.00	23.55	B
ATOM	2982	O	ASN	263	19.316	51.006	23.369	1.00	18.90	B
ATOM	2983	N	HIS	264	17.958	49.279	22.900	1.00	23.91	B
ATOM	2984	H	HIS	264	17.341	48.618	23.274	1.00	0.00	B
ATOM	2985	CA	HIS	264	18.189	49.276	21.458	1.00	26.11	B
ATOM	2986	CB	HIS	264	17.205	48.308	20.778	1.00	23.47	B
ATOM	2987	CG	HIS	264	15.766	48.685	20.947	1.00	22.25	B
ATOM	2988	CD2	HIS	264	14.846	48.294	21.863	1.00	24.90	B
ATOM	2989	ND1	HIS	264	15.129	49.594	20.131	1.00	23.90	B
ATOM	2990	HD1	HIS	264	15.530	50.056	19.366	1.00	0.00	B
ATOM	2991	CE1	HIS	264	13.881	49.748	20.532	1.00	31.00	B
ATOM	2992	NE2	HIS	264	13.683	48.970	21.586	1.00	28.44	B
ATOM	2993	HE2	HIS	264	12.847	48.889	22.081	1.00	0.00	B
ATOM	2994	C	HIS	264	18.163	50.601	20.706	1.00	29.92	B
ATOM	2995	O	HIS	264	18.712	50.710	19.614	1.00	31.12	B
ATOM	2996	N	ARG	265	17.527	51.613	21.282	1.00	30.38	B
ATOM	2997	H	ARG	265	17.125	51.493	22.161	1.00	0.00	B
ATOM	2998	CA	ARG	265	17.435	52.905	20.619	1.00	33.48	B
ATOM	2999	CB	ARG	265	16.140	53.580	21.011	1.00	35.96	B
ATOM	3000	CG	ARG	265	14.909	52.909	20.585	1.00	43.13	B
ATOM	3001	CD	ARG	265	14.090	53.926	19.852	1.00	45.62	B

ATOM	3002	NE	ARG	265	13.403	54.838	20.755	1.00	41.09	B
ATOM	3003	HE	ARG	265	13.054	54.478	21.594	1.00	0.00	B
ATOM	3004	CZ	ARG	265	13.218	56.130	20.506	1.00	42.46	B
ATOM	3005	NH1	ARG	265	13.671	56.670	19.380	1.00	43.62	B
ATOM	3006	HH11	ARG	265	14.151	56.104	18.710	1.00	0.00	B
ATOM	3007	HH12	ARG	265	13.529	57.644	19.202	1.00	0.00	B
ATOM	3008	NH2	ARG	265	12.565	56.879	21.374	1.00	43.11	B
ATOM	3009	HH21	ARG	265	12.206	56.472	22.213	1.00	0.00	B
ATOM	3010	HH22	ARG	265	12.426	57.852	21.189	1.00	0.00	B
ATOM	3011	C	ARG	265	18.535	53.875	21.040	1.00	31.98	B
ATOM	3012	O	ARG	265	18.666	54.954	20.443	1.00	25.36	B
ATOM	3013	N	LEU	266	19.302	53.472	22.059	1.00	27.18	B
ATOM	3014	H	LEU	266	19.231	52.547	22.360	1.00	0.00	B
ATOM	3015	CA	LEU	266	20.303	54.346	22.685	1.00	26.54	B
ATOM	3016	CB	LEU	266	20.987	53.646	23.864	1.00	21.25	B
ATOM	3017	CG	LEU	266	20.178	53.787	25.158	1.00	23.40	B
ATOM	3018	CD1	LEU	266	20.950	53.117	26.265	1.00	16.18	B
ATOM	3019	CD2	LEU	266	19.900	55.260	25.505	1.00	27.07	B
ATOM	3020	C	LEU	266	21.337	54.990	21.809	1.00	28.09	B
ATOM	3021	O	LEU	266	21.467	56.208	21.838	1.00	30.85	B
ATOM	3022	N	GLN	267	22.045	54.199	21.031	1.00	29.76	B
ATOM	3023	H	GLN	267	21.873	53.236	21.016	1.00	0.00	B
ATOM	3024	CA	GLN	267	23.086	54.733	20.162	1.00	29.56	B
ATOM	3025	CB	GLN	267	23.692	53.605	19.344	1.00	36.52	B
ATOM	3026	CG	GLN	267	23.964	52.362	20.169	1.00	50.23	B
ATOM	3027	CD	GLN	267	23.778	51.084	19.380	1.00	58.15	B
ATOM	3028	OE1	GLN	267	23.350	50.056	19.919	1.00	60.56	B
ATOM	3029	NE2	GLN	267	24.100	51.138	18.089	1.00	62.36	B
ATOM	3030	HE21	GLN	267	24.434	51.976	17.706	1.00	0.00	B
ATOM	3031	HE22	GLN	267	23.988	50.324	17.561	1.00	0.00	B
ATOM	3032	C	GLN	267	22.556	55.825	19.245	1.00	31.18	B
ATOM	3033	O	GLN	267	23.145	56.905	19.130	1.00	27.34	B
ATOM	3034	N	LYS	268	21.443	55.540	18.582	1.00	29.62	B
ATOM	3035	H	LYS	268	21.009	54.672	18.704	1.00	0.00	B
ATOM	3036	CA	LYS	268	20.872	56.514	17.687	1.00	26.36	B
ATOM	3037	CB	LYS	268	19.650	55.937	16.976	1.00	29.19	B
ATOM	3038	CG	LYS	268	19.037	56.897	15.952	1.00	37.26	B
ATOM	3039	CD	LYS	268	20.002	57.194	14.800	1.00	37.93	B
ATOM	3040	CE	LYS	268	19.555	56.514	13.516	1.00	45.23	B
ATOM	3041	NZ	LYS	268	20.397	56.862	12.327	1.00	50.96	B
ATOM	3042	HZ1	LYS	268	21.379	56.574	12.501	1.00	0.00	B
ATOM	3043	HZ2	LYS	268	20.358	57.888	12.163	1.00	0.00	B
ATOM	3044	HZ3	LYS	268	20.032	56.365	11.488	1.00	0.00	B
ATOM	3045	C	LYS	268	20.476	57.755	18.464	1.00	22.33	B
ATOM	3046	O	LYS	268	20.834	58.864	18.085	1.00	18.43	B
ATOM	3047	N	VAL	269	19.744	57.570	19.556	1.00	25.38	B
ATOM	3048	H	VAL	269	19.505	56.659	19.828	1.00	0.00	B
ATOM	3049	CA	VAL	269	19.294	58.706	20.357	1.00	24.60	B
ATOM	3050	CB	VAL	269	18.422	58.270	21.562	1.00	21.43	B
ATOM	3051	CG1	VAL	269	18.359	59.395	22.582	1.00	20.07	B
ATOM	3052	CG2	VAL	269	17.014	57.926	21.092	1.00	13.06	B
ATOM	3053	C	VAL	269	20.471	59.518	20.876	1.00	25.36	B
ATOM	3054	O	VAL	269	20.453	60.753	20.827	1.00	24.64	B
ATOM	3055	N	ILE	270	21.494	58.830	21.372	1.00	25.28	B
ATOM	3056	H	ILE	270	21.457	57.854	21.397	1.00	0.00	B
ATOM	3057	CA	ILE	270	22.674	59.520	21.878	1.00	20.75	B
ATOM	3058	CB	ILE	270	23.657	58.535	22.568	1.00	22.70	B
ATOM	3059	CG2	ILE	270	25.019	59.210	22.813	1.00	16.22	B
ATOM	3060	CG1	ILE	270	23.078	58.064	23.912	1.00	27.60	B
ATOM	3061	CD1	ILE	270	21.829	58.794	24.368	1.00	28.95	B
ATOM	3062	C	ILE	270	23.377	60.244	20.730	1.00	24.26	B
ATOM	3063	O	ILE	270	23.877	61.350	20.919	1.00	25.59	B
ATOM	3064	N	GLN	271	23.387	59.646	19.538	1.00	24.44	B
ATOM	3065	H	GLN	271	22.937	58.783	19.424	1.00	0.00	B
ATOM	3066	CA	GLN	271	24.066	60.269	18.389	1.00	24.78	B
ATOM	3067	CB	GLN	271	24.125	59.335	17.186	1.00	22.72	B
ATOM	3068	CG	GLN	271	24.955	59.918	16.040	1.00	26.49	B
ATOM	3069	CD	GLN	271	26.371	60.238	16.481	1.00	29.28	B
ATOM	3070	OE1	GLN	271	26.939	61.274	16.127	1.00	30.26	B
ATOM	3071	NE2	GLN	271	26.951	59.345	17.264	1.00	30.30	B
ATOM	3072	HE21	GLN	271	26.460	58.535	17.522	1.00	0.00	B
ATOM	3073	HE22	GLN	271	27.862	59.527	17.562	1.00	0.00	B
ATOM	3074	C	GLN	271	23.404	61.550	17.944	1.00	24.46	B

ATOM	3075	O	GLN	271	24.067	62.496	17.509	1.00	16.78	B
ATOM	3076	N	ASP	272	22.082	61.557	18.025	1.00	21.10	B
ATOM	3077	H	ASP	272	21.615	60.756	18.343	1.00	0.00	B
ATOM	3078	CA	ASP	272	21.325	62.718	17.650	1.00	17.66	B
ATOM	3079	CB	ASP	272	19.848	62.340	17.563	1.00	21.71	B
ATOM	3080	CG	ASP	272	19.567	61.417	16.376	1.00	24.50	B
ATOM	3081	OD1	ASP	272	20.276	61.541	15.361	1.00	31.04	B
ATOM	3082	OD2	ASP	272	18.656	60.571	16.449	1.00	28.77	B
ATOM	3083	C	ASP	272	21.593	63.832	18.656	1.00	17.80	B
ATOM	3084	O	ASP	272	21.699	64.997	18.284	1.00	18.02	B
ATOM	3085	N	CYS	273	21.729	63.477	19.931	1.00	18.60	B
ATOM	3086	H	CYS	273	21.636	62.537	20.187	1.00	0.00	B
ATOM	3087	CA	CYS	273	22.022	64.488	20.945	1.00	20.63	B
ATOM	3088	CB	CYS	273	22.050	63.867	22.347	1.00	16.54	B
ATOM	3089	SG	CYS	273	20.445	63.515	23.095	1.00	35.11	B
ATOM	3090	C	CYS	273	23.396	65.085	20.641	1.00	23.93	B
ATOM	3091	O	CYS	273	23.579	66.305	20.707	1.00	21.34	B
ATOM	3092	N	GLU	274	24.346	64.212	20.304	1.00	21.52	B
ATOM	3093	H	GLU	274	24.114	63.261	20.261	1.00	0.00	B
ATOM	3094	CA	GLU	274	25.723	64.601	19.993	1.00	25.93	B
ATOM	3095	CB	GLU	274	26.523	63.355	19.575	1.00	25.37	B
ATOM	3096	CG	GLU	274	28.017	63.412	19.847	1.00	33.76	B
ATOM	3097	CD	GLU	274	28.381	64.114	21.149	1.00	35.86	B
ATOM	3098	OE1	GLU	274	29.384	64.855	21.154	1.00	39.26	B
ATOM	3099	OE2	GLU	274	27.682	63.929	22.164	1.00	31.65	B
ATOM	3100	C	GLU	274	25.801	65.667	18.896	1.00	27.29	B
ATOM	3101	O	GLU	274	26.479	66.692	19.055	1.00	21.91	B
ATOM	3102	N	ASP	275	25.110	65.409	17.786	1.00	25.89	B
ATOM	3103	H	ASP	275	24.605	64.571	17.736	1.00	0.00	B
ATOM	3104	CA	ASP	275	25.069	66.319	16.635	1.00	29.31	B
ATOM	3105	CB	ASP	275	24.320	65.655	15.471	1.00	28.05	B
ATOM	3106	CG	ASP	275	25.031	64.420	14.938	1.00	37.38	B
ATOM	3107	OD1	ASP	275	26.257	64.293	15.145	1.00	41.51	B
ATOM	3108	OD2	ASP	275	24.360	63.575	14.305	1.00	34.32	B
ATOM	3109	C	ASP	275	24.408	67.674	16.939	1.00	29.09	B
ATOM	3110	O	ASP	275	24.678	68.679	16.268	1.00	22.13	B
ATOM	3111	N	GLU	276	23.529	67.688	17.935	1.00	30.74	B
ATOM	3112	H	GLU	276	23.353	66.859	18.423	1.00	0.00	B
ATOM	3113	CA	GLU	276	22.817	68.901	18.327	1.00	32.15	B
ATOM	3114	CB	GLU	276	21.403	68.554	18.792	1.00	31.31	B
ATOM	3115	CG	GLU	276	20.404	68.622	17.654	1.00	35.70	B
ATOM	3116	CD	GLU	276	19.015	68.175	18.049	1.00	42.31	B
ATOM	3117	OE1	GLU	276	18.415	67.389	17.284	1.00	40.50	B
ATOM	3118	OE2	GLU	276	18.521	68.606	19.115	1.00	46.76	B
ATOM	3119	C	GLU	276	23.606	69.557	19.431	1.00	29.44	B
ATOM	3120	O	GLU	276	23.234	70.604	19.968	1.00	24.35	B
ATOM	3121	N	ASN	277	24.727	68.918	19.744	1.00	28.11	B
ATOM	3122	H	ASN	277	24.942	68.087	19.272	1.00	0.00	B
ATOM	3123	CA	ASN	277	25.644	69.401	20.757	1.00	29.61	B
ATOM	3124	CB	ASN	277	26.309	70.682	20.271	1.00	32.09	B
ATOM	3125	CG	ASN	277	27.387	70.398	19.252	1.00	38.92	B
ATOM	3126	OD1	ASN	277	28.455	69.880	19.597	1.00	38.13	B
ATOM	3127	ND2	ASN	277	27.113	70.712	17.989	1.00	39.28	B
ATOM	3128	HD21	ASN	277	26.245	71.104	17.760	1.00	0.00	B
ATOM	3129	HD22	ASN	277	27.804	70.534	17.319	1.00	0.00	B
ATOM	3130	C	ASN	277	25.023	69.617	22.111	1.00	27.06	B
ATOM	3131	O	ASN	277	25.118	70.691	22.693	1.00	28.18	B
ATOM	3132	N	ILE	278	24.390	68.572	22.613	1.00	22.45	B
ATOM	3133	H	ILE	278	24.339	67.740	22.096	1.00	0.00	B
ATOM	3134	CA	ILE	278	23.775	68.640	23.909	1.00	18.31	B
ATOM	3135	CB	ILE	278	22.422	67.904	23.899	1.00	14.49	B
ATOM	3136	CG2	ILE	278	21.895	67.787	25.306	1.00	12.68	B
ATOM	3137	CG1	ILE	278	21.454	68.639	22.962	1.00	17.11	B
ATOM	3138	CD1	ILE	278	20.093	68.024	22.870	1.00	16.07	B
ATOM	3139	C	ILE	278	24.728	67.978	24.903	1.00	18.85	B
ATOM	3140	O	ILE	278	25.052	66.802	24.767	1.00	17.29	B
ATOM	3141	N	GLN	279	25.180	68.738	25.896	1.00	15.07	B
ATOM	3142	H	GLN	279	24.907	69.676	25.956	1.00	0.00	B
ATOM	3143	CA	GLN	279	26.071	68.182	26.891	1.00	20.54	B
ATOM	3144	CB	GLN	279	26.788	69.299	27.636	1.00	22.04	B
ATOM	3145	CG	GLN	279	28.008	68.836	28.428	1.00	25.39	B
ATOM	3146	CD	GLN	279	28.683	69.984	29.146	1.00	25.91	B
ATOM	3147	OE1	GLN	279	29.500	69.777	30.040	1.00	26.55	B

ATOM	3148	NE2	GLN	279	28.340	71.208	28.758	1.00	23.93	B
ATOM	3149	HE21	GLN	279	27.685	71.328	28.040	1.00	0.00	B
ATOM	3150	HE22	GLN	279	28.769	71.963	29.211	1.00	0.00	B
ATOM	3151	C	GLN	279	25.253	67.347	27.866	1.00	17.77	B
ATOM	3152	O	GLN	279	24.310	67.847	28.475	1.00	21.13	B
ATOM	3153	N	ARG	280	25.620	66.081	28.025	1.00	19.35	B
ATOM	3154	H	ARG	280	26.398	65.742	27.538	1.00	0.00	B
ATOM	3155	CA	ARG	280	24.880	65.184	28.913	1.00	17.76	B
ATOM	3156	CB	ARG	280	24.285	64.007	28.123	1.00	13.32	B
ATOM	3157	CG	ARG	280	24.065	64.255	26.641	1.00	16.90	B
ATOM	3158	CD	ARG	280	23.912	62.956	25.872	1.00	12.99	B
ATOM	3159	NE	ARG	280	25.175	62.404	25.368	1.00	14.94	B
ATOM	3160	HE	ARG	280	25.533	61.605	25.802	1.00	0.00	B
ATOM	3161	CZ	ARG	280	25.866	62.931	24.363	1.00	18.57	B
ATOM	3162	NH1	ARG	280	25.421	64.025	23.754	1.00	16.91	B
ATOM	3163	HH11	ARG	280	24.569	64.453	24.058	1.00	0.00	B
ATOM	3164	HH12	ARG	280	25.937	64.421	22.996	1.00	0.00	B
ATOM	3165	NH2	ARG	280	27.005	62.370	23.965	1.00	12.64	B
ATOM	3166	HH21	ARG	280	27.344	61.552	24.430	1.00	0.00	B
ATOM	3167	HH22	ARG	280	27.521	62.763	23.211	1.00	0.00	B
ATOM	3168	C	ARG	280	25.628	64.601	30.111	1.00	16.54	B
ATOM	3169	O	ARG	280	26.644	63.912	29.968	1.00	18.85	B
ATOM	3170	N	PHE	281	25.099	64.893	31.288	1.00	14.11	B
ATOM	3171	H	PHE	281	24.324	65.492	31.315	1.00	0.00	B
ATOM	3172	CA	PHE	281	25.611	64.374	32.543	1.00	13.98	B
ATOM	3173	CB	PHE	281	25.610	65.452	33.632	1.00	20.05	B
ATOM	3174	CG	PHE	281	26.572	66.572	33.394	1.00	23.08	B
ATOM	3175	CD1	PHE	281	26.213	67.660	32.606	1.00	22.44	B
ATOM	3176	CD2	PHE	281	27.822	66.564	33.998	1.00	20.52	B
ATOM	3177	CE1	PHE	281	27.086	68.732	32.426	1.00	23.69	B
ATOM	3178	CE2	PHE	281	28.702	67.628	33.826	1.00	19.90	B
ATOM	3179	CZ	PHE	281	28.328	68.718	33.038	1.00	22.07	B
ATOM	3180	C	PHE	281	24.570	63.306	32.929	1.00	16.85	B
ATOM	3181	O	PHE	281	23.370	63.589	32.962	1.00	17.22	B
ATOM	3182	N	SER	282	25.022	62.095	33.231	1.00	14.65	B
ATOM	3183	H	SER	282	25.984	61.920	33.203	1.00	0.00	B
ATOM	3184	CA	SER	282	24.104	61.030	33.605	1.00	14.06	B
ATOM	3185	CB	SER	282	24.152	59.884	32.578	1.00	11.06	B
ATOM	3186	OG	SER	282	25.449	59.298	32.482	1.00	18.85	B
ATOM	3187	HG	SER	282	25.433	58.594	31.836	1.00	0.00	B
ATOM	3188	C	SER	282	24.449	60.516	34.984	1.00	15.44	B
ATOM	3189	O	SER	282	25.631	60.359	35.310	1.00	22.28	B
ATOM	3190	N	ILE	283	23.413	60.278	35.787	1.00	16.47	B
ATOM	3191	H	ILE	283	22.513	60.444	35.442	1.00	0.00	B
ATOM	3192	CA	ILE	283	23.541	59.776	37.152	1.00	12.03	B
ATOM	3193	CB	ILE	283	22.870	60.730	38.164	1.00	13.63	B
ATOM	3194	CG2	ILE	283	22.863	60.095	39.532	1.00	11.53	B
ATOM	3195	CG1	ILE	283	23.606	62.072	38.237	1.00	18.66	B
ATOM	3196	CD1	ILE	283	23.280	63.039	37.120	1.00	14.72	B
ATOM	3197	C	ILE	283	22.842	58.403	37.283	1.00	20.66	B
ATOM	3198	O	ILE	283	21.623	58.291	37.068	1.00	19.36	B
ATOM	3199	N	ALA	284	23.617	57.369	37.616	1.00	18.27	B
ATOM	3200	H	ALA	284	24.579	57.514	37.731	1.00	0.00	B
ATOM	3201	CA	ALA	284	23.082	56.022	37.814	1.00	16.02	B
ATOM	3202	CB	ALA	284	24.000	54.974	37.196	1.00	17.51	B
ATOM	3203	C	ALA	284	22.963	55.767	39.299	1.00	18.28	B
ATOM	3204	O	ALA	284	23.956	55.892	40.018	1.00	22.88	B
ATOM	3205	N	ILE	285	21.753	55.430	39.764	1.00	19.46	B
ATOM	3206	H	ILE	285	21.001	55.378	39.139	1.00	0.00	B
ATOM	3207	CA	ILE	285	21.523	55.137	41.182	1.00	20.18	B
ATOM	3208	CB	ILE	285	20.188	55.716	41.703	1.00	19.17	B
ATOM	3209	CG2	ILE	285	19.893	55.174	43.103	1.00	17.01	B
ATOM	3210	CG1	ILE	285	20.256	57.235	41.762	1.00	17.37	B
ATOM	3211	CD1	ILE	285	19.131	57.923	41.023	1.00	18.02	B
ATOM	3212	C	ILE	285	21.469	53.621	41.280	1.00	20.23	B
ATOM	3213	O	ILE	285	20.615	52.986	40.659	1.00	20.26	B
ATOM	3214	N	LEU	286	22.384	53.045	42.052	1.00	17.07	B
ATOM	3215	H	LEU	286	23.012	53.610	42.549	1.00	0.00	B
ATOM	3216	CA	LEU	286	22.471	51.602	42.176	1.00	19.43	B
ATOM	3217	CB	LEU	286	23.949	51.171	42.263	1.00	19.07	B
ATOM	3218	CG	LEU	286	25.035	51.649	41.276	1.00	17.49	B
ATOM	3219	CD1	LEU	286	25.830	50.442	40.797	1.00	12.99	B
ATOM	3220	CD2	LEU	286	24.431	52.420	40.099	1.00	10.34	B

ATOM	3221	C	LEU	286	21.722	51.058	43.382	1.00	21.59	B
ATOM	3222	O	LEU	286	21.885	49.895	43.742	1.00	23.43	B
ATOM	3223	N	GLY	287	20.899	51.903	43.997	1.00	21.97	B
ATOM	3224	H	GLY	287	20.792	52.812	43.647	1.00	0.00	B
ATOM	3225	CA	GLY	287	20.158	51.493	45.173	1.00	19.38	B
ATOM	3226	C	GLY	287	19.312	50.236	45.051	1.00	23.15	B
ATOM	3227	O	GLY	287	19.575	49.221	45.708	1.00	20.35	B
ATOM	3228	N	HIS	288	18.285	50.308	44.215	1.00	17.51	B
ATOM	3229	H	HIS	288	18.130	51.137	43.713	1.00	0.00	B
ATOM	3230	CA	HIS	288	17.387	49.196	44.027	1.00	14.47	B
ATOM	3231	CB	HIS	288	16.298	49.571	43.042	1.00	14.52	B
ATOM	3232	CG	HIS	288	15.289	48.495	42.825	1.00	15.66	B
ATOM	3233	CD2	HIS	288	15.157	47.585	41.826	1.00	6.58	B
ATOM	3234	ND1	HIS	288	14.289	48.220	43.731	1.00	10.26	B
ATOM	3235	HD1	HIS	288	14.116	48.715	44.551	1.00	0.00	B
ATOM	3236	CE1	HIS	288	13.575	47.198	43.293	1.00	16.43	B
ATOM	3237	NE2	HIS	288	14.083	46.794	42.141	1.00	11.36	B
ATOM	3238	HE2	HIS	288	13.751	46.056	41.599	1.00	0.00	B
ATOM	3239	C	HIS	288	18.086	47.939	43.532	1.00	20.49	B
ATOM	3240	O	HIS	288	17.786	46.833	43.982	1.00	21.10	B
ATOM	3241	N	TYR	289	19.007	48.117	42.595	1.00	20.56	B
ATOM	3242	H	TYR	289	19.202	49.023	42.276	1.00	0.00	B
ATOM	3243	CA	TYR	289	19.733	46.995	42.034	1.00	18.95	B
ATOM	3244	CB	TYR	289	20.740	47.489	41.004	1.00	16.43	B
ATOM	3245	CG	TYR	289	20.221	47.446	39.597	1.00	16.33	B
ATOM	3246	CD1	TYR	289	19.048	48.104	39.264	1.00	14.79	B
ATOM	3247	CE1	TYR	289	18.563	48.086	37.978	1.00	23.36	B
ATOM	3248	CD2	TYR	289	20.907	46.757	38.592	1.00	18.79	B
ATOM	3249	CE2	TYR	289	20.428	46.733	37.287	1.00	18.41	B
ATOM	3250	CZ	TYR	289	19.252	47.409	36.991	1.00	22.68	B
ATOM	3251	OH	TYR	289	18.755	47.437	35.716	1.00	18.85	B
ATOM	3252	HH	TYR	289	17.943	47.954	35.703	1.00	0.00	B
ATOM	3253	C	TYR	289	20.467	46.221	43.120	1.00	16.62	B
ATOM	3254	O	TYR	289	20.383	44.995	43.190	1.00	16.84	B
ATOM	3255	N	ASN	290	21.182	46.940	43.976	1.00	14.38	B
ATOM	3256	H	ASN	290	21.203	47.921	43.912	1.00	0.00	B
ATOM	3257	CA	ASN	290	21.927	46.254	45.007	1.00	16.73	B
ATOM	3258	CB	ASN	290	23.029	47.167	45.546	1.00	16.82	B
ATOM	3259	CG	ASN	290	24.202	47.282	44.575	1.00	23.04	B
ATOM	3260	OD1	ASN	290	24.477	46.361	43.788	1.00	17.55	B
ATOM	3261	ND2	ASN	290	24.892	48.410	44.618	1.00	21.77	B
ATOM	3262	HD21	ASN	290	24.637	49.116	45.247	1.00	0.00	B
ATOM	3263	HD22	ASN	290	25.647	48.501	44.001	1.00	0.00	B
ATOM	3264	C	ASN	290	21.016	45.733	46.110	1.00	18.43	B
ATOM	3265	O	ASN	290	21.301	44.698	46.720	1.00	15.23	B
ATOM	3266	N	ARG	291	19.909	46.434	46.330	1.00	16.92	B
ATOM	3267	H	ARG	291	19.744	47.244	45.805	1.00	0.00	B
ATOM	3268	CA	ARG	291	18.926	46.034	47.336	1.00	21.23	B
ATOM	3269	CB	ARG	291	17.804	47.089	47.452	1.00	24.15	B
ATOM	3270	CG	ARG	291	17.983	48.113	48.576	1.00	25.81	B
ATOM	3271	CD	ARG	291	17.245	49.456	48.310	1.00	34.39	B
ATOM	3272	NE	ARG	291	16.026	49.348	47.505	1.00	42.57	B
ATOM	3273	HE	ARG	291	15.575	48.480	47.481	1.00	0.00	B
ATOM	3274	CZ	ARG	291	15.478	50.349	46.806	1.00	43.67	B
ATOM	3275	NH1	ARG	291	16.035	51.551	46.803	1.00	38.72	B
ATOM	3276	HH11	ARG	291	16.864	51.719	47.331	1.00	0.00	B
ATOM	3277	HH12	ARG	291	15.620	52.293	46.275	1.00	0.00	B
ATOM	3278	NH2	ARG	291	14.356	50.148	46.110	1.00	39.35	B
ATOM	3279	HH21	ARG	291	13.920	49.248	46.114	1.00	0.00	B
ATOM	3280	HH22	ARG	291	13.952	50.897	45.585	1.00	0.00	B
ATOM	3281	C	ARG	291	18.337	44.690	46.908	1.00	10.17	B
ATOM	3282	O	ARG	291	17.966	43.883	47.734	1.00	10.79	B
ATOM	3283	N	GLY	292	18.283	44.442	45.607	1.00	18.23	B
ATOM	3284	H	GLY	292	18.625	45.096	44.967	1.00	0.00	B
ATOM	3285	CA	GLY	292	17.712	43.187	45.139	1.00	19.17	B
ATOM	3286	C	GLY	292	18.625	42.170	44.468	1.00	20.74	B
ATOM	3287	O	GLY	292	18.143	41.280	43.759	1.00	16.44	B
ATOM	3288	N	ASN	293	19.925	42.262	44.724	1.00	19.28	B
ATOM	3289	H	ASN	293	20.235	42.945	45.353	1.00	0.00	B
ATOM	3290	CA	ASN	293	20.918	41.375	44.101	1.00	23.38	B
ATOM	3291	CB	ASN	293	20.855	39.945	44.650	1.00	21.82	B
ATOM	3292	CG	ASN	293	22.109	39.122	44.279	1.00	28.61	B
ATOM	3293	OD1	ASN	293	22.011	38.021	43.727	1.00	20.89	B

```
ATOM   3294  ND2 ASN   293      23.286  39.667  44.580  1.00 16.64      B
ATOM   3295 HD21 ASN   293      23.321  40.544  45.016  1.00  0.00      B
ATOM   3296 HD22 ASN   293      24.090  39.158  44.353  1.00  0.00      B
ATOM   3297  C   ASN   293      20.851  41.290  42.578  1.00 24.68      B
ATOM   3298  O   ASN   293      20.937  40.199  42.009  1.00 25.78      B
ATOM   3299  N   LEU   294      20.690  42.432  41.917  1.00 27.45      B
ATOM   3300  H   LEU   294      20.582  43.268  42.415  1.00  0.00      B
ATOM   3301  CA  LEU   294      20.666  42.454  40.457  1.00 26.46      B
ATOM   3302  CB  LEU   294      19.696  43.514  39.920  1.00 21.98      B
ATOM   3303  CG  LEU   294      18.249  43.549  40.402  1.00 33.38      B
ATOM   3304  CD1 LEU   294      17.464  44.534  39.538  1.00 32.24      B
ATOM   3305  CD2 LEU   294      17.639  42.177  40.334  1.00 27.44      B
ATOM   3306  C   LEU   294      22.063  42.822  39.984  1.00 24.21      B
ATOM   3307  O   LEU   294      22.709  43.685  40.571  1.00 23.66      B
ATOM   3308  N   SER   295      22.526  42.174  38.924  1.00 23.08      B
ATOM   3309  H   SER   295      21.984  41.469  38.512  1.00  0.00      B
ATOM   3310  CA  SER   295      23.833  42.497  38.366  1.00 24.49      B
ATOM   3311  CB  SER   295      24.211  41.481  37.284  1.00 22.71      B
ATOM   3312  OG  SER   295      25.057  42.058  36.307  1.00 28.77      B
ATOM   3313  HG  SER   295      25.856  42.370  36.726  1.00  0.00      B
ATOM   3314  C   SER   295      23.724  43.909  37.759  1.00 20.29      B
ATOM   3315  O   SER   295      22.815  44.187  36.983  1.00 18.00      B
ATOM   3316  N   THR   296      24.660  44.777  38.118  1.00 16.49      B
ATOM   3317  H   THR   296      25.372  44.479  38.724  1.00  0.00      B
ATOM   3318  CA  THR   296      24.679  46.166  37.653  1.00 18.66      B
ATOM   3319  CB  THR   296      25.023  47.101  38.804  1.00 19.68      B
ATOM   3320  OG1 THR   296      26.258  46.675  39.393  1.00 19.06      B
ATOM   3321  HG1 THR   296      26.162  45.778  39.722  1.00  0.00      B
ATOM   3322  CG2 THR   296      23.927  47.060  39.863  1.00 22.45      B
ATOM   3323  C   THR   296      25.664  46.470  36.535  1.00 19.63      B
ATOM   3324  O   THR   296      25.808  47.626  36.136  1.00 17.70      B
ATOM   3325  N   GLU   297      26.324  45.439  36.016  1.00 21.20      B
ATOM   3326  H   GLU   297      26.131  44.536  36.341  1.00  0.00      B
ATOM   3327  CA  GLU   297      27.325  45.622  34.972  1.00 21.26      B
ATOM   3328  CB  GLU   297      28.042  44.291  34.710  1.00 30.39      B
ATOM   3329  CG  GLU   297      29.004  43.863  35.838  1.00 39.46      B
ATOM   3330  CD  GLU   297      28.305  43.191  37.015  1.00 41.75      B
ATOM   3331  OE1 GLU   297      27.330  42.455  36.778  1.00 45.39      B
ATOM   3332  OE2 GLU   297      28.735  43.392  38.173  1.00 35.85      B
ATOM   3333  C   GLU   297      26.789  46.210  33.675  1.00 22.11      B
ATOM   3334  O   GLU   297      27.344  47.184  33.151  1.00 18.94      B
ATOM   3335  N   LYS   298      25.717  45.622  33.153  1.00 15.26      B
ATOM   3336  H   LYS   298      25.330  44.845  33.608  1.00  0.00      B
ATOM   3337  CA  LYS   298      25.105  46.107  31.925  1.00 17.69      B
ATOM   3338  CB  LYS   298      23.958  45.163  31.500  1.00 22.54      B
ATOM   3339  CG  LYS   298      23.297  45.486  30.151  1.00 16.04      B
ATOM   3340  CD  LYS   298      22.093  44.565  29.903  1.00 15.19      B
ATOM   3341  CE  LYS   298      21.795  44.409  28.415  1.00 24.32      B
ATOM   3342  NZ  LYS   298      20.353  44.064  28.147  1.00 31.08      B
ATOM   3343 HZ1 LYS   298      19.741  44.822  28.518  1.00  0.00      B
ATOM   3344 HZ2 LYS   298      20.114  43.169  28.620  1.00  0.00      B
ATOM   3345 HZ3 LYS   298      20.202  43.968  27.124  1.00  0.00      B
ATOM   3346  C   LYS   298      24.556  47.506  32.172  1.00 14.71      B
ATOM   3347  O   LYS   298      24.718  48.410  31.356  1.00 19.72      B
ATOM   3348  N   PHE   299      23.915  47.659  33.322  1.00 19.20      B
ATOM   3349  H   PHE   299      23.860  46.891  33.929  1.00  0.00      B
ATOM   3350  CA  PHE   299      23.283  48.912  33.744  1.00 16.23      B
ATOM   3351  CB  PHE   299      22.600  48.673  35.110  1.00 15.69      B
ATOM   3352  CG  PHE   299      22.135  49.920  35.826  1.00 17.83      B
ATOM   3353  CD1 PHE   299      21.724  51.058  35.127  1.00 17.90      B
ATOM   3354  CD2 PHE   299      22.110  49.949  37.216  1.00 17.55      B
ATOM   3355  CE1 PHE   299      21.303  52.191  35.802  1.00 15.38      B
ATOM   3356  CE2 PHE   299      21.687  51.087  37.897  1.00 26.58      B
ATOM   3357  CZ  PHE   299      21.282  52.213  37.179  1.00 19.56      B
ATOM   3358  C   PHE   299      24.276  50.079  33.818  1.00 17.61      B
ATOM   3359  O   PHE   299      24.087  51.099  33.163  1.00 16.95      B
ATOM   3360  N   VAL   300      25.327  49.914  34.617  1.00 17.22      B
ATOM   3361  H   VAL   300      25.433  49.066  35.094  1.00  0.00      B
ATOM   3362  CA  VAL   300      26.322  50.959  34.801  1.00 18.55      B
ATOM   3363  CB  VAL   300      27.421  50.492  35.773  1.00 16.60      B
ATOM   3364  CG1 VAL   300      28.724  51.220  35.492  1.00 21.52      B
ATOM   3365  CG2 VAL   300      26.974  50.723  37.195  1.00 19.24      B
ATOM   3366  C   VAL   300      26.941  51.382  33.480  1.00 17.23      B
```

ATOM	3367	O	VAL	300	27.075	52.569	33.198	1.00	15.55	B
ATOM	3368	N	GLU	301	27.293	50.400	32.665	1.00	15.45	B
ATOM	3369	H	GLU	301	27.145	49.471	32.939	1.00	0.00	B
ATOM	3370	CA	GLU	301	27.892	50.674	31.374	1.00	20.07	B
ATOM	3371	CB	GLU	301	28.282	49.349	30.708	1.00	25.34	B
ATOM	3372	CG	GLU	301	28.738	49.477	29.274	1.00	40.60	B
ATOM	3373	CD	GLU	301	27.589	49.413	28.283	1.00	50.61	B
ATOM	3374	OE1	GLU	301	26.510	48.871	28.633	1.00	56.16	B
ATOM	3375	OE2	GLU	301	27.771	49.908	27.146	1.00	54.98	B
ATOM	3376	C	GLU	301	26.956	51.483	30.457	1.00	22.33	B
ATOM	3377	O	GLU	301	27.413	52.316	29.663	1.00	18.68	B
ATOM	3378	N	GLU	302	25.652	51.235	30.573	1.00	21.56	B
ATOM	3379	H	GLU	302	25.349	50.566	31.221	1.00	0.00	B
ATOM	3380	CA	GLU	302	24.655	51.931	29.759	1.00	19.52	B
ATOM	3381	CB	GLU	302	23.316	51.173	29.825	1.00	23.59	B
ATOM	3382	CG	GLU	302	22.069	51.902	29.281	1.00	26.77	B
ATOM	3383	CD	GLU	302	20.820	51.024	29.367	1.00	19.66	B
ATOM	3384	OE1	GLU	302	20.836	49.919	28.798	1.00	15.94	B
ATOM	3385	OE2	GLU	302	19.836	51.428	30.010	1.00	19.29	B
ATOM	3386	C	GLU	302	24.487	53.409	30.163	1.00	13.52	B
ATOM	3387	O	GLU	302	24.426	54.276	29.303	1.00	17.34	B
ATOM	3388	N	ILE	303	24.419	53.710	31.452	1.00	17.66	B
ATOM	3389	H	ILE	303	24.459	53.009	32.135	1.00	0.00	B
ATOM	3390	CA	ILE	303	24.282	55.117	31.825	1.00	15.73	B
ATOM	3391	CB	ILE	303	24.030	55.310	33.330	1.00	18.32	B
ATOM	3392	CG2	ILE	303	23.348	56.686	33.566	1.00	12.98	B
ATOM	3393	CG1	ILE	303	23.163	54.164	33.864	1.00	21.47	B
ATOM	3394	CD1	ILE	303	21.731	54.137	33.322	1.00	24.44	B
ATOM	3395	C	ILE	303	25.575	55.848	31.452	1.00	20.62	B
ATOM	3396	O	ILE	303	25.542	57.005	31.051	1.00	22.42	B
ATOM	3397	N	LYS	304	26.715	55.172	31.593	1.00	17.68	B
ATOM	3398	H	LYS	304	26.703	54.253	31.932	1.00	0.00	B
ATOM	3399	CA	LYS	304	27.980	55.805	31.236	1.00	22.51	B
ATOM	3400	CB	LYS	304	29.183	54.907	31.567	1.00	13.79	B
ATOM	3401	CG	LYS	304	30.528	55.611	31.424	1.00	27.58	B
ATOM	3402	CD	LYS	304	31.449	55.355	32.617	1.00	29.45	B
ATOM	3403	CE	LYS	304	32.745	56.172	32.533	1.00	33.25	B
ATOM	3404	NZ	LYS	304	33.272	56.638	33.870	1.00	32.84	B
ATOM	3405	HZ1	LYS	304	33.470	55.816	34.473	1.00	0.00	B
ATOM	3406	HZ2	LYS	304	32.561	57.243	34.330	1.00	0.00	B
ATOM	3407	HZ3	LYS	304	34.147	57.184	33.727	1.00	0.00	B
ATOM	3408	C	LYS	304	27.963	56.096	29.745	1.00	20.33	B
ATOM	3409	O	LYS	304	28.455	57.130	29.307	1.00	21.96	B
ATOM	3410	N	SER	305	27.376	55.185	28.977	1.00	16.80	B
ATOM	3411	H	SER	305	26.990	54.387	29.393	1.00	0.00	B
ATOM	3412	CA	SER	305	27.295	55.346	27.534	1.00	20.13	B
ATOM	3413	CB	SER	305	26.662	54.112	26.898	1.00	18.58	B
ATOM	3414	OG	SER	305	25.453	54.454	26.253	1.00	30.77	B
ATOM	3415	HG	SER	305	25.630	55.103	25.567	1.00	0.00	B
ATOM	3416	C	SER	305	26.517	56.584	27.107	1.00	15.70	B
ATOM	3417	O	SER	305	26.679	57.045	25.991	1.00	14.73	B
ATOM	3418	N	ILE	306	25.677	57.110	27.994	1.00	20.28	B
ATOM	3419	H	ILE	306	25.593	56.689	28.877	1.00	0.00	B
ATOM	3420	CA	ILE	306	24.872	58.299	27.698	1.00	14.20	B
ATOM	3421	CB	ILE	306	23.555	58.269	28.527	1.00	25.18	B
ATOM	3422	CG2	ILE	306	22.895	59.661	28.591	1.00	18.61	B
ATOM	3423	CG1	ILE	306	22.588	57.265	27.900	1.00	23.41	B
ATOM	3424	CD1	ILE	306	22.204	56.151	28.834	1.00	19.11	B
ATOM	3425	C	ILE	306	25.656	59.594	27.985	1.00	18.43	B
ATOM	3426	O	ILE	306	25.481	60.596	27.301	1.00	15.22	B
ATOM	3427	N	ALA	307	26.522	59.555	28.996	1.00	20.05	B
ATOM	3428	H	ALA	307	26.607	58.727	29.512	1.00	0.00	B
ATOM	3429	CA	ALA	307	27.350	60.711	29.369	1.00	21.87	B
ATOM	3430	CB	ALA	307	28.291	60.341	30.515	1.00	13.67	B
ATOM	3431	C	ALA	307	28.177	61.271	28.226	1.00	15.95	B
ATOM	3432	O	ALA	307	28.653	60.542	27.370	1.00	18.44	B
ATOM	3433	N	SER	308	28.343	62.583	28.231	1.00	18.17	B
ATOM	3434	H	SER	308	27.907	63.117	28.925	1.00	0.00	B
ATOM	3435	CA	SER	308	29.154	63.252	27.225	1.00	19.58	B
ATOM	3436	CB	SER	308	28.962	64.759	27.306	1.00	15.23	B
ATOM	3437	OG	SER	308	27.810	65.168	26.610	1.00	22.22	B
ATOM	3438	HG	SER	308	27.890	64.920	25.685	1.00	0.00	B
ATOM	3439	C	SER	308	30.606	62.935	27.556	1.00	16.69	B

	ATOM	3440	O	SER	308	30.930	62.608	28.691	1.00	19.32	B
	ATOM	3441	N	GLU	309	31.478	63.027	26.570	1.00	19.87	B
	ATOM	3442	H	GLU	309	31.181	63.264	25.667	1.00	0.00	B
	ATOM	3443	CA	GLU	309	32.883	62.772	26.840	1.00	27.15	B
5	ATOM	3444	CB	GLU	309	33.576	62.254	25.586	1.00	30.43	B
	ATOM	3445	CG	GLU	309	33.735	60.743	25.594	1.00	42.04	B
	ATOM	3446	CD	GLU	309	33.305	60.100	24.293	1.00	51.38	B
	ATOM	3447	OE1	GLU	309	33.438	58.860	24.165	1.00	53.41	B
	ATOM	3448	OE2	GLU	309	32.836	60.835	23.398	1.00	53.07	B
10	ATOM	3449	C	GLU	309	33.549	64.049	27.339	1.00	23.13	B
	ATOM	3450	O	GLU	309	33.260	65.147	26.859	1.00	24.83	B
	ATOM	3451	N	PRO	310	34.429	63.934	28.339	1.00	22.49	B
	ATOM	3452	CD	PRO	310	35.090	65.153	28.838	1.00	22.94	B
	ATOM	3453	CA	PRO	310	34.873	62.730	29.061	1.00	20.46	B
15	ATOM	3454	CB	PRO	310	36.043	63.238	29.899	1.00	21.98	B
	ATOM	3455	CG	PRO	310	35.744	64.692	30.108	1.00	22.65	B
	ATOM	3456	C	PRO	310	33.789	62.122	29.952	1.00	20.72	B
	ATOM	3457	O	PRO	310	33.170	62.840	30.748	1.00	21.32	B
	ATOM	3458	N	THR	311	33.557	60.813	29.833	1.00	16.53	B
20	ATOM	3459	H	THR	311	34.066	60.282	29.184	1.00	0.00	B
	ATOM	3460	CA	THR	311	32.556	60.172	30.669	1.00	20.30	B
	ATOM	3461	CB	THR	311	32.387	58.671	30.367	1.00	26.73	B
	ATOM	3462	OG1	THR	311	33.656	58.018	30.481	1.00	33.48	B
	ATOM	3463	HG1	THR	311	33.997	58.128	31.371	1.00	0.00	B
25	ATOM	3464	CG2	THR	311	31.798	58.449	28.983	1.00	27.71	B
	ATOM	3465	C	THR	311	32.894	60.277	32.153	1.00	25.27	B
	ATOM	3466	O	THR	311	32.022	60.561	32.960	1.00	29.95	B
	ATOM	3467	N	GLU	312	34.153	60.052	32.524	1.00	24.13	B
	ATOM	3468	H	GLU	312	34.837	59.854	31.852	1.00	0.00	B
30	ATOM	3469	CA	GLU	312	34.509	60.104	33.940	1.00	27.24	B
	ATOM	3470	CB	GLU	312	36.004	59.840	34.153	1.00	30.20	B
	ATOM	3471	CG	GLU	312	36.889	60.121	32.953	1.00	44.57	B
	ATOM	3472	CD	GLU	312	36.932	58.966	31.967	1.00	42.06	B
	ATOM	3473	OE1	GLU	312	37.286	57.844	32.376	1.00	44.27	B
35	ATOM	3474	OE2	GLU	312	36.609	59.188	30.778	1.00	45.67	B
	ATOM	3475	C	GLU	312	34.116	61.425	34.590	1.00	28.79	B
	ATOM	3476	O	GLU	312	33.898	61.483	35.803	1.00	25.09	B
	ATOM	3477	N	LYS	313	34.028	62.485	33.795	1.00	26.01	B
	ATOM	3478	H	LYS	313	34.229	62.399	32.840	1.00	0.00	B
40	ATOM	3479	CA	LYS	313	33.635	63.776	34.340	1.00	24.40	B
	ATOM	3480	CB	LYS	313	34.311	64.904	33.563	1.00	29.52	B
	ATOM	3481	CG	LYS	313	35.760	65.150	33.989	1.00	40.92	B
	ATOM	3482	CD	LYS	313	35.838	66.011	35.246	1.00	42.61	B
	ATOM	3483	CE	LYS	313	37.263	66.454	35.516	1.00	44.08	B
45	ATOM	3484	NZ	LYS	313	37.340	67.390	36.668	1.00	45.93	B
	ATOM	3485	HZ1	LYS	313	36.977	66.918	37.522	1.00	0.00	B
	ATOM	3486	HZ2	LYS	313	36.767	68.234	36.469	1.00	0.00	B
	ATOM	3487	HZ3	LYS	313	38.329	67.670	36.822	1.00	0.00	B
	ATOM	3488	C	LYS	313	32.114	63.968	34.305	1.00	23.67	B
50	ATOM	3489	O	LYS	313	31.546	64.615	35.183	1.00	21.16	B
	ATOM	3490	N	HIS	314	31.462	63.394	33.299	1.00	17.77	B
	ATOM	3491	H	HIS	314	31.956	62.860	32.643	1.00	0.00	B
	ATOM	3492	CA	HIS	314	30.026	63.546	33.163	1.00	23.14	B
	ATOM	3493	CB	HIS	314	29.664	63.688	31.681	1.00	23.44	B
55	ATOM	3494	CG	HIS	314	30.242	64.916	31.035	1.00	26.47	B
	ATOM	3495	CD2	HIS	314	31.317	65.073	30.226	1.00	24.55	B
	ATOM	3496	ND1	HIS	314	29.652	66.157	31.136	1.00	27.43	B
	ATOM	3497	HD1	HIS	314	28.867	66.359	31.682	1.00	0.00	B
	ATOM	3498	CE1	HIS	314	30.344	67.031	30.426	1.00	13.83	B
60	ATOM	3499	NE2	HIS	314	31.355	66.398	29.864	1.00	30.72	B
	ATOM	3500	HE2	HIS	314	32.021	66.817	29.289	1.00	0.00	B
	ATOM	3501	C	HIS	314	29.178	62.430	33.812	1.00	19.97	B
	ATOM	3502	O	HIS	314	28.022	62.663	34.133	1.00	15.17	B
	ATOM	3503	N	PHE	315	29.752	61.245	34.019	1.00	12.58	B
65	ATOM	3504	H	PHE	315	30.680	61.109	33.753	1.00	0.00	B
	ATOM	3505	CA	PHE	315	29.018	60.139	34.637	1.00	11.72	B
	ATOM	3506	CB	PHE	315	29.435	58.799	34.022	1.00	13.63	B
	ATOM	3507	CG	PHE	315	28.821	57.595	34.702	1.00	17.15	B
	ATOM	3508	CD1	PHE	315	27.427	57.409	34.716	1.00	12.18	B
70	ATOM	3509	CD2	PHE	315	29.626	56.635	35.320	1.00	21.49	B
	ATOM	3510	CE1	PHE	315	26.856	56.290	35.330	1.00	15.00	B
	ATOM	3511	CE2	PHE	315	29.052	55.501	35.941	1.00	19.73	B
	ATOM	3512	CZ	PHE	315	27.651	55.337	35.943	1.00	11.10	B

ATOM	3513	C	PHE	315	29.189	60.045	36.153	1.00	20.36	B
ATOM	3514	O	PHE	315	30.307	60.141	36.672	1.00	18.84	B
ATOM	3515	N	PHE	316	28.074	59.844	36.863	1.00	23.38	B
ATOM	3516	H	PHE	316	27.214	59.795	36.398	1.00	0.00	B
ATOM	3517	CA	PHE	316	28.107	59.697	38.317	1.00	14.23	B
ATOM	3518	CB	PHE	316	27.395	60.853	39.002	1.00	19.22	B
ATOM	3519	CG	PHE	316	28.065	62.188	38.810	1.00	27.88	B
ATOM	3520	CD1	PHE	316	27.744	62.994	37.721	1.00	28.03	B
ATOM	3521	CD2	PHE	316	28.969	62.675	39.754	1.00	31.78	B
ATOM	3522	CE1	PHE	316	28.306	64.271	37.578	1.00	29.90	B
ATOM	3523	CE2	PHE	316	29.535	63.959	39.609	1.00	25.22	B
ATOM	3524	CZ	PHE	316	29.195	64.746	38.523	1.00	25.24	B
ATOM	3525	C	PHE	316	27.453	58.392	38.737	1.00	19.30	B
ATOM	3526	O	PHE	316	26.306	58.100	38.370	1.00	16.18	B
ATOM	3527	N	ASN	317	28.194	57.593	39.489	1.00	22.70	B
ATOM	3528	H	ASN	317	29.106	57.868	39.725	1.00	0.00	B
ATOM	3529	CA	ASN	317	27.695	56.312	39.979	1.00	23.24	B
ATOM	3530	CB	ASN	317	28.741	55.210	39.759	1.00	22.04	B
ATOM	3531	CG	ASN	317	28.335	53.871	40.391	1.00	25.87	B
ATOM	3532	OD1	ASN	317	27.738	53.828	41.467	1.00	26.08	B
ATOM	3533	ND2	ASN	317	28.658	52.778	39.716	1.00	13.17	B
ATOM	3534	HD21	ASN	317	29.130	52.855	38.858	1.00	0.00	B
ATOM	3535	HD22	ASN	317	28.407	51.916	40.103	1.00	0.00	B
ATOM	3536	C	ASN	317	27.410	56.484	41.463	1.00	18.96	B
ATOM	3537	O	ASN	317	28.326	56.476	42.277	1.00	21.45	B
ATOM	3538	N	VAL	318	26.142	56.669	41.804	1.00	23.81	B
ATOM	3539	H	VAL	318	25.458	56.678	41.102	1.00	0.00	B
ATOM	3540	CA	VAL	318	25.731	56.857	43.187	1.00	20.00	B
ATOM	3541	CB	VAL	318	24.576	57.902	43.272	1.00	21.73	B
ATOM	3542	CG1	VAL	318	23.466	57.514	42.335	1.00	27.34	B
ATOM	3543	CG2	VAL	318	24.060	58.012	44.688	1.00	15.43	B
ATOM	3544	C	VAL	318	25.280	55.508	43.737	1.00	20.44	B
ATOM	3545	O	VAL	318	24.488	54.814	43.108	1.00	17.67	B
ATOM	3546	N	SER	319	25.797	55.133	44.903	1.00	20.29	B
ATOM	3547	H	SER	319	26.417	55.731	45.369	1.00	0.00	B
ATOM	3548	CA	SER	319	25.455	53.840	45.502	1.00	17.71	B
ATOM	3549	CB	SER	319	26.268	53.608	46.775	1.00	13.81	B
ATOM	3550	OG	SER	319	27.123	54.701	47.038	1.00	31.29	B
ATOM	3551	HG	SER	319	26.599	55.496	47.151	1.00	0.00	B
ATOM	3552	C	SER	319	23.969	53.697	45.816	1.00	18.64	B
ATOM	3553	O	SER	319	23.382	52.644	45.575	1.00	16.85	B
ATOM	3554	N	ASP	320	23.361	54.745	46.351	1.00	16.38	B
ATOM	3555	H	ASP	320	23.866	55.566	46.537	1.00	0.00	B
ATOM	3556	CA	ASP	320	21.943	54.679	46.665	1.00	20.08	B
ATOM	3557	CB	ASP	320	21.720	53.772	47.878	1.00	26.71	B
ATOM	3558	CG	ASP	320	22.310	54.337	49.143	1.00	23.52	B
ATOM	3559	OD1	ASP	320	23.287	55.104	49.059	1.00	27.09	B
ATOM	3560	OD2	ASP	320	21.791	54.013	50.227	1.00	27.50	B
ATOM	3561	C	ASP	320	21.317	56.062	46.886	1.00	16.45	B
ATOM	3562	O	ASP	320	22.018	57.062	47.037	1.00	15.80	B
ATOM	3563	N	GLU	321	19.991	56.088	46.902	1.00	14.19	B
ATOM	3564	H	GLU	321	19.508	55.238	46.818	1.00	0.00	B
ATOM	3565	CA	GLU	321	19.220	57.313	47.037	1.00	21.02	B
ATOM	3566	CB	GLU	321	17.738	56.966	47.233	1.00	12.70	B
ATOM	3567	CG	GLU	321	17.115	56.285	46.017	1.00	12.53	B
ATOM	3568	CD	GLU	321	17.187	54.767	46.098	1.00	17.82	B
ATOM	3569	OE1	GLU	321	17.982	54.231	46.903	1.00	14.77	B
ATOM	3570	OE2	GLU	321	16.439	54.103	45.355	1.00	17.04	B
ATOM	3571	C	GLU	321	19.675	58.272	48.130	1.00	24.90	B
ATOM	3572	O	GLU	321	19.749	59.480	47.906	1.00	22.58	B
ATOM	3573	N	LEU	322	19.967	57.732	49.307	1.00	26.45	B
ATOM	3574	H	LEU	322	19.881	56.763	49.428	1.00	0.00	B
ATOM	3575	CA	LEU	322	20.411	58.550	50.425	1.00	28.16	B
ATOM	3576	CB	LEU	322	20.477	57.707	51.709	1.00	32.06	B
ATOM	3577	CG	LEU	322	19.155	57.600	52.478	1.00	34.11	B
ATOM	3578	CD1	LEU	322	19.357	56.923	53.839	1.00	29.26	B
ATOM	3579	CD2	LEU	322	18.583	59.000	52.645	1.00	30.30	B
ATOM	3580	C	LEU	322	21.768	59.193	50.154	1.00	30.66	B
ATOM	3581	O	LEU	322	22.119	60.195	50.776	1.00	33.88	B
ATOM	3582	N	ALA	323	22.527	58.625	49.219	1.00	26.52	B
ATOM	3583	H	ALA	323	22.199	57.828	48.752	1.00	0.00	B
ATOM	3584	CA	ALA	323	23.839	59.166	48.886	1.00	24.47	B
ATOM	3585	CB	ALA	323	24.772	58.030	48.451	1.00	19.17	B

ATOM	3586	C	ALA	323	23.832	60.283	47.820	1.00	24.00	B
ATOM	3587	O	ALA	323	24.829	60.971	47.657	1.00	24.66	B
ATOM	3588	N	LEU	324	22.735	60.481	47.096	1.00	21.81	B
ATOM	3589	H	LEU	324	21.941	59.928	47.248	1.00	0.00	B
ATOM	3590	CA	LEU	324	22.715	61.534	46.069	1.00	19.68	B
ATOM	3591	CB	LEU	324	21.312	61.715	45.508	1.00	18.39	B
ATOM	3592	CG	LEU	324	20.899	60.637	44.519	1.00	13.78	B
ATOM	3593	CD1	LEU	324	19.402	60.611	44.457	1.00	16.65	B
ATOM	3594	CD2	LEU	324	21.511	60.908	43.143	1.00	14.31	B
ATOM	3595	C	LEU	324	23.226	62.892	46.561	1.00	23.65	B
ATOM	3596	O	LEU	324	23.938	63.594	45.841	1.00	18.23	B
ATOM	3597	N	VAL	325	22.852	63.264	47.783	1.00	26.30	B
ATOM	3598	H	VAL	325	22.272	62.672	48.305	1.00	0.00	B
ATOM	3599	CA	VAL	325	23.282	64.533	48.369	1.00	31.91	B
ATOM	3600	CB	VAL	325	22.778	64.643	49.837	1.00	37.44	B
ATOM	3601	CG1	VAL	325	23.583	65.687	50.609	1.00	34.83	B
ATOM	3602	CG2	VAL	325	21.294	65.008	49.843	1.00	42.56	B
ATOM	3603	C	VAL	325	24.819	64.710	48.330	1.00	30.26	B
ATOM	3604	O	VAL	325	25.327	65.825	48.398	1.00	32.04	B
ATOM	3605	N	THR	326	25.548	63.609	48.194	1.00	28.75	B
ATOM	3606	H	THR	326	25.094	62.744	48.113	1.00	0.00	B
ATOM	3607	CA	THR	326	26.998	63.657	48.167	1.00	31.17	B
ATOM	3608	CB	THR	326	27.607	62.288	48.511	1.00	27.84	B
ATOM	3609	OG1	THR	326	27.229	61.332	47.514	1.00	34.82	B
ATOM	3610	HG1	THR	326	26.277	61.260	47.489	1.00	0.00	B
ATOM	3611	CG2	THR	326	27.136	61.826	49.880	1.00	30.51	B
ATOM	3612	C	THR	326	27.608	64.128	46.856	1.00	32.05	B
ATOM	3613	O	THR	326	28.745	64.590	46.846	1.00	30.58	B
ATOM	3614	N	ILE	327	26.879	64.002	45.750	1.00	33.07	B
ATOM	3615	H	ILE	327	25.984	63.603	45.793	1.00	0.00	B
ATOM	3616	CA	ILE	327	27.421	64.461	44.472	1.00	32.83	B
ATOM	3617	CB	ILE	327	27.185	63.446	43.300	1.00	35.01	B
ATOM	3618	CG2	ILE	327	27.881	62.118	43.604	1.00	32.57	B
ATOM	3619	CG1	ILE	327	25.691	63.252	43.048	1.00	35.05	B
ATOM	3620	CD1	ILE	327	25.371	62.796	41.633	1.00	32.92	B
ATOM	3621	C	ILE	327	26.852	65.814	44.061	1.00	30.01	B
ATOM	3622	O	ILE	327	27.211	66.348	43.011	1.00	23.73	B
ATOM	3623	N	VAL	328	25.972	66.370	44.894	1.00	26.90	B
ATOM	3624	H	VAL	328	25.715	65.896	45.711	1.00	0.00	B
ATOM	3625	CA	VAL	328	25.383	67.675	44.600	1.00	32.68	B
ATOM	3626	CB	VAL	328	24.535	68.177	45.798	1.00	36.74	B
ATOM	3627	CG1	VAL	328	24.075	69.612	45.561	1.00	29.92	B
ATOM	3628	CG2	VAL	328	23.332	67.265	45.998	1.00	30.30	B
ATOM	3629	C	VAL	328	26.451	68.741	44.255	1.00	33.15	B
ATOM	3630	O	VAL	328	26.310	69.477	43.279	1.00	35.10	B
ATOM	3631	N	LYS	329	27.528	68.801	45.038	1.00	32.80	B
ATOM	3632	H	LYS	329	27.613	68.169	45.781	1.00	0.00	B
ATOM	3633	CA	LYS	329	28.585	69.789	44.819	1.00	31.42	B
ATOM	3634	CB	LYS	329	29.563	69.773	45.990	1.00	38.34	B
ATOM	3635	CG	LYS	329	29.794	71.139	46.623	1.00	42.75	B
ATOM	3636	CD	LYS	329	29.245	71.201	48.053	1.00	46.58	B
ATOM	3637	CE	LYS	329	27.716	71.275	48.078	1.00	48.13	B
ATOM	3638	NZ	LYS	329	27.089	70.078	48.711	1.00	48.31	B
ATOM	3639	HZ1	LYS	329	27.420	69.992	49.693	1.00	0.00	B
ATOM	3640	HZ2	LYS	329	27.357	69.225	48.180	1.00	0.00	B
ATOM	3641	HZ3	LYS	329	26.055	70.182	48.701	1.00	0.00	B
ATOM	3642	C	LYS	329	29.365	69.648	43.517	1.00	29.75	B
ATOM	3643	O	LYS	329	29.548	70.633	42.791	1.00	30.62	B
ATOM	3644	N	ALA	330	29.818	68.434	43.226	1.00	27.05	B
ATOM	3645	H	ALA	330	29.623	67.699	43.844	1.00	0.00	B
ATOM	3646	CA	ALA	330	30.598	68.145	42.022	1.00	27.52	B
ATOM	3647	CB	ALA	330	31.094	66.683	42.058	1.00	15.14	B
ATOM	3648	C	ALA	330	29.804	68.397	40.742	1.00	24.45	B
ATOM	3649	O	ALA	330	30.282	69.043	39.811	1.00	29.53	B
ATOM	3650	N	LEU	331	28.585	67.878	40.708	1.00	27.74	B
ATOM	3651	H	LEU	331	28.266	67.372	41.483	1.00	0.00	B
ATOM	3652	CA	LEU	331	27.701	68.040	39.555	1.00	26.77	B
ATOM	3653	CB	LEU	331	26.398	67.267	39.771	1.00	20.69	B
ATOM	3654	CG	LEU	331	25.594	66.834	38.543	1.00	27.56	B
ATOM	3655	CD1	LEU	331	24.126	67.117	38.817	1.00	32.10	B
ATOM	3656	CD2	LEU	331	26.079	67.540	37.280	1.00	22.24	B
ATOM	3657	C	LEU	331	27.358	69.497	39.326	1.00	14.45	B
ATOM	3658	O	LEU	331	27.376	69.973	38.209	1.00	25.05	B

```
ATOM   3659  N   GLY   332      27.036  70.199  40.400  1.00 20.98      B
ATOM   3660  H   GLY   332      27.036  69.772  41.280  1.00  0.00      B
ATOM   3661  CA  GLY   332      26.683  71.599  40.277  1.00 16.97      B
ATOM   3662  C   GLY   332      27.830  72.431  39.740  1.00 23.19      B
ATOM   3663  O   GLY   332      27.611  73.389  39.000  1.00 20.06      B
ATOM   3664  N   GLU   333      29.063  72.086  40.102  1.00 22.14      B
ATOM   3665  H   GLU   333      29.218  71.324  40.699  1.00  0.00      B
ATOM   3666  CA  GLU   333      30.169  72.870  39.589  1.00 28.24      B
ATOM   3667  CB  GLU   333      31.358  72.859  40.557  1.00 33.30      B
ATOM   3668  CG  GLU   333      31.779  71.505  41.068  1.00 40.29      B
ATOM   3669  CD  GLU   333      33.065  71.595  41.866  1.00 46.24      B
ATOM   3670  OE1 GLU   333      34.122  71.152  41.350  1.00 45.00      B
ATOM   3671  OE2 GLU   333      33.008  72.121  43.006  1.00 38.74      B
ATOM   3672  C   GLU   333      30.594  72.407  38.206  1.00 27.85      B
ATOM   3673  O   GLU   333      31.048  73.215  37.397  1.00 29.71      B
ATOM   3674  N   ARG   334      30.438  71.115  37.920  1.00 25.03      B
ATOM   3675  H   ARG   334      30.079  70.508  38.601  1.00  0.00      B
ATOM   3676  CA  ARG   334      30.799  70.594  36.602  1.00 18.82      B
ATOM   3677  CB  ARG   334      30.839  69.062  36.610  1.00 17.45      B
ATOM   3678  CG  ARG   334      32.187  68.485  36.951  1.00 12.28      B
ATOM   3679  CD  ARG   334      32.112  66.986  37.157  1.00 20.12      B
ATOM   3680  NE  ARG   334      33.151  66.520  38.065  1.00 26.33      B
ATOM   3681  HE  ARG   334      33.835  67.163  38.343  1.00  0.00      B
ATOM   3682  CZ  ARG   334      33.230  65.281  38.543  1.00 33.67      B
ATOM   3683  NH1 ARG   334      32.321  64.366  38.200  1.00 28.50      B
ATOM   3684  HH11 ARG   334      31.575  64.611  37.583  1.00  0.00      B
ATOM   3685  HH12 ARG   334      32.388  63.437  38.563  1.00  0.00      B
ATOM   3686  NH2 ARG   334      34.220  64.956  39.364  1.00 33.01      B
ATOM   3687  HH21 ARG   334      34.901  65.642  39.624  1.00  0.00      B
ATOM   3688  HH22 ARG   334      34.287  64.026  39.728  1.00  0.00      B
ATOM   3689  C   ARG   334      29.811  71.057  35.532  1.00 16.42      B
ATOM   3690  O   ARG   334      30.185  71.277  34.383  1.00 17.09      B
ATOM   3691  N   ILE   335      28.541  71.184  35.889  1.00 18.26      B
ATOM   3692  H   ILE   335      28.256  70.974  36.802  1.00  0.00      B
ATOM   3693  CA  ILE   335      27.574  71.640  34.899  1.00 21.52      B
ATOM   3694  CB  ILE   335      26.166  71.818  35.518  1.00 22.25      B
ATOM   3695  CG2 ILE   335      26.288  72.266  36.946  1.00 30.01      B
ATOM   3696  CG1 ILE   335      25.365  72.886  34.776  1.00 13.73      B
ATOM   3697  CD1 ILE   335      25.018  72.533  33.362  1.00 25.02      B
ATOM   3698  C   ILE   335      28.053  72.976  34.345  1.00 24.47      B
ATOM   3699  O   ILE   335      28.012  73.203  33.135  1.00 23.62      B
ATOM   3700  N   PHE   336      28.537  73.841  35.235  1.00 24.00      B
ATOM   3701  H   PHE   336      28.593  73.575  36.176  1.00  0.00      B
ATOM   3702  CA  PHE   336      28.987  75.179  34.848  1.00 29.92      B
ATOM   3703  CB  PHE   336      28.561  76.179  35.932  1.00 31.59      B
ATOM   3704  CG  PHE   336      27.077  76.412  35.973  1.00 26.05      B
ATOM   3705  CD1 PHE   336      26.290  75.810  36.955  1.00 30.05      B
ATOM   3706  CD2 PHE   336      26.459  77.184  34.993  1.00 24.28      B
ATOM   3707  CE1 PHE   336      24.895  75.970  36.958  1.00 25.70      B
ATOM   3708  CE2 PHE   336      25.072  77.353  34.981  1.00 26.15      B
ATOM   3709  CZ  PHE   336      24.287  76.738  35.971  1.00 22.17      B
ATOM   3710  C   PHE   336      30.463  75.384  34.495  1.00 31.44      B
ATOM   3711  O   PHE   336      30.870  76.491  34.124  1.00 27.91      B
ATOM   3712  N   ALA   337      31.260  74.328  34.583  1.00 30.25      B
ATOM   3713  H   ALA   337      30.895  73.465  34.875  1.00  0.00      B
ATOM   3714  CA  ALA   337      32.674  74.440  34.253  1.00 35.57      B
ATOM   3715  CB  ALA   337      33.518  74.124  35.479  1.00 31.23      B
ATOM   3716  C   ALA   337      33.085  73.537  33.083  1.00 38.16      B
ATOM   3717  O   ALA   337      33.755  73.989  32.162  1.00 40.82      B
ATOM   3718  N   LEU   338      32.668  72.271  33.125  1.00 41.05      B
ATOM   3719  H   LEU   338      32.114  71.987  33.880  1.00  0.00      B
ATOM   3720  CA  LEU   338      33.003  71.286  32.092  1.00 43.90      B
ATOM   3721  CB  LEU   338      32.334  69.943  32.405  1.00 43.75      B
ATOM   3722  CG  LEU   338      33.195  68.796  32.939  1.00 46.43      B
ATOM   3723  CD1 LEU   338      32.356  67.526  33.010  1.00 48.40      B
ATOM   3724  CD2 LEU   338      34.406  68.586  32.043  1.00 46.34      B
ATOM   3725  C   LEU   338      32.609  71.712  30.683  1.00 47.43      B
ATOM   3726  O   LEU   338      33.390  71.430  29.740  1.00 47.18      B
ATOM   3727  OT  LEU   338      31.518  72.308  30.541  1.00 50.73      B
ATOM   3728  OH2 H2O     1      11.763  72.942  27.999  1.00 13.08      W
ATOM   3729  H1  H2O     1      12.196  72.994  27.149  1.00  0.00      W
ATOM   3730  H2  H2O     1      11.929  72.051  28.302  1.00  0.00      W
ATOM   3731  OH2 H2O     2      33.606  75.805  28.263  1.00 38.72      W
```

	ATOM	3732	H1	H2O	2	33.652	75.559	29.186	1.00	0.00	W
	ATOM	3733	H2	H2O	2	33.674	76.762	28.267	1.00	0.00	W
	ATOM	3734	OH2	H2O	3	46.772	76.583	-1.078	1.00	59.42	W
	ATOM	3735	H1	H2O	3	46.862	77.129	-1.859	1.00	0.00	W
5	ATOM	3736	H2	H2O	3	47.663	76.280	-0.894	1.00	0.00	W
	ATOM	3737	OH2	H2O	4	17.892	53.996	32.616	1.00	12.25	W
	ATOM	3738	H1	H2O	4	17.234	54.300	31.991	1.00	0.00	W
	ATOM	3739	H2	H2O	4	17.561	53.146	32.907	1.00	0.00	W
	ATOM	3740	OH2	H2O	5	28.607	56.204	23.823	1.00	37.75	W
10	ATOM	3741	H1	H2O	5	27.946	56.312	24.504	1.00	0.00	W
	ATOM	3742	H2	H2O	5	29.014	57.067	23.742	1.00	0.00	W
	ATOM	3743	OH2	H2O	6	33.273	78.294	33.342	1.00	29.21	W
	ATOM	3744	H1	H2O	6	32.852	77.437	33.359	1.00	0.00	W
	ATOM	3745	H2	H2O	6	32.646	78.878	33.776	1.00	0.00	W
15	ATOM	3746	OH2	H2O	7	17.238	53.571	16.889	1.00	44.25	W
	ATOM	3747	H1	H2O	7	16.904	53.246	16.055	1.00	0.00	W
	ATOM	3748	H2	H2O	7	17.520	52.787	17.360	1.00	0.00	W
	ATOM	3749	OH2	H2O	8	13.870	78.571	33.824	1.00	15.18	W
	ATOM	3750	H1	H2O	8	13.855	78.968	34.695	1.00	0.00	W
20	ATOM	3751	H2	H2O	8	13.148	79.001	33.357	1.00	0.00	W
	ATOM	3752	OH2	H2O	9	25.865	90.956	-20.487	1.00	31.46	W
	ATOM	3753	H1	H2O	9	25.185	90.524	-21.011	1.00	0.00	W
	ATOM	3754	H2	H2O	9	25.994	90.377	-19.740	1.00	0.00	W
	ATOM	3755	OH2	H2O	10	36.614	69.921	37.968	1.00	47.49	W
25	ATOM	3756	H1	H2O	10	37.012	69.641	38.786	1.00	0.00	W
	ATOM	3757	H2	H2O	10	37.218	69.613	37.294	1.00	0.00	W
	ATOM	3758	OH2	H2O	11	25.295	79.036	26.770	1.00	27.54	W
	ATOM	3759	H1	H2O	11	24.707	79.474	26.157	1.00	0.00	W
	ATOM	3760	H2	H2O	11	24.928	79.225	27.628	1.00	0.00	W
30	ATOM	3761	OH2	H2O	12	18.365	40.699	50.184	1.00	18.35	W
	ATOM	3762	H1	H2O	12	17.417	40.675	50.306	1.00	0.00	W
	ATOM	3763	H2	H2O	12	18.696	39.974	50.712	1.00	0.00	W
	ATOM	3764	OH2	H2O	13	21.562	51.184	21.243	1.00	25.48	W
	ATOM	3765	H1	H2O	13	21.072	51.974	21.467	1.00	0.00	W
35	ATOM	3766	H2	H2O	13	21.182	50.500	21.792	1.00	0.00	W
	ATOM	3767	OH2	H2O	14	7.521	51.792	47.594	1.00	15.43	W
	ATOM	3768	H1	H2O	14	7.094	51.205	46.975	1.00	0.00	W
	ATOM	3769	H2	H2O	14	8.187	52.245	47.075	1.00	0.00	W
	ATOM	3770	OH2	H2O	15	10.086	64.032	53.718	1.00	28.77	W
40	ATOM	3771	H1	H2O	15	9.359	63.736	53.165	1.00	0.00	W
	ATOM	3772	H2	H2O	15	10.701	63.300	53.713	1.00	0.00	W
	ATOM	3773	OH2	H2O	16	35.315	54.724	34.014	1.00	42.64	W
	ATOM	3774	H1	H2O	16	36.015	55.349	33.832	1.00	0.00	W
	ATOM	3775	H2	H2O	16	35.680	54.137	34.676	1.00	0.00	W
45	ATOM	3776	OH2	H2O	17	6.402	69.762	21.688	1.00	32.95	W
	ATOM	3777	H1	H2O	17	6.183	70.430	22.334	1.00	0.00	W
	ATOM	3778	H2	H2O	17	6.335	70.208	20.844	1.00	0.00	W
	ATOM	3779	OH2	H2O	18	14.632	41.929	43.654	1.00	18.32	W
	ATOM	3780	H1	H2O	18	15.167	42.282	44.368	1.00	0.00	W
50	ATOM	3781	H2	H2O	18	15.258	41.449	43.107	1.00	0.00	W
	ATOM	3782	OH2	H2O	19	40.329	91.816	-7.396	1.00	25.37	W
	ATOM	3783	H1	H2O	19	39.913	91.345	-6.675	1.00	0.00	W
	ATOM	3784	H2	H2O	19	40.631	92.636	-7.004	1.00	0.00	W
	ATOM	3785	OH2	H2O	20	6.640	73.014	46.415	1.00	33.60	W
55	ATOM	3786	H1	H2O	20	6.738	72.084	46.624	1.00	0.00	W
	ATOM	3787	H2	H2O	20	6.989	73.098	45.531	1.00	0.00	W
	ATOM	3788	OH2	H2O	21	37.583	68.788	40.034	1.00	36.96	W
	ATOM	3789	H1	H2O	21	37.026	69.000	39.287	1.00	0.00	W
	ATOM	3790	H2	H2O	21	38.300	68.285	39.657	1.00	0.00	W
60	ATOM	3791	OH2	H2O	22	5.165	71.647	48.591	1.00	35.16	W
	ATOM	3792	H1	H2O	22	5.385	70.721	48.682	1.00	0.00	W
	ATOM	3793	H2	H2O	22	4.625	71.844	49.355	1.00	0.00	W
	ATOM	3794	OH2	H2O	23	22.348	84.835	16.567	1.00	16.19	W
	ATOM	3795	H1	H2O	23	23.280	84.637	16.464	1.00	0.00	W
65	ATOM	3796	H2	H2O	23	22.114	85.295	15.758	1.00	0.00	W
	ATOM	3797	OH2	H2O	24	15.889	49.740	39.303	1.00	19.38	W
	ATOM	3798	H1	H2O	24	16.319	48.932	39.026	1.00	0.00	W
	ATOM	3799	H2	H2O	24	15.010	49.471	39.561	1.00	0.00	W
	ATOM	3800	OH2	H2O	25	37.655	61.332	27.513	1.00	31.70	W
70	ATOM	3801	H1	H2O	25	36.886	61.727	27.931	1.00	0.00	W
	ATOM	3802	H2	H2O	25	37.861	60.575	28.057	1.00	0.00	W
	ATOM	3803	OH2	H2O	26	17.980	71.537	17.982	1.00	39.05	W
	ATOM	3804	H1	H2O	26	17.960	70.901	17.268	1.00	0.00	W

ATOM	3805	H2	H2O	26	18.160	71.014	18.764	1.00	0.00	W
ATOM	3806	OH2	H2O	27	12.412	74.571	-14.438	1.00	54.13	W
ATOM	3807	H1	H2O	27	11.645	74.040	-14.647	1.00	0.00	W
ATOM	3808	H2	H2O	27	12.947	74.009	-13.875	1.00	0.00	W
ATOM	3809	OH2	H2O	28	35.093	93.688	9.513	1.00	49.07	W
ATOM	3810	H1	H2O	28	34.158	93.901	9.502	1.00	0.00	W
ATOM	3811	H2	H2O	28	35.143	92.843	9.955	1.00	0.00	W
ATOM	3812	OH2	H2O	29	27.557	67.319	47.587	1.00	20.63	W
ATOM	3813	H1	H2O	29	28.387	67.684	47.271	1.00	0.00	W
ATOM	3814	H2	H2O	29	27.650	66.377	47.466	1.00	0.00	W
ATOM	3815	OH2	H2O	30	12.145	50.693	37.668	1.00	22.09	W
ATOM	3816	H1	H2O	30	12.508	49.987	38.209	1.00	0.00	W
ATOM	3817	H2	H2O	30	12.370	51.493	38.131	1.00	0.00	W
ATOM	3818	OH2	H2O	31	29.496	59.286	42.408	1.00	37.05	W
ATOM	3819	H1	H2O	31	30.012	59.213	43.211	1.00	0.00	W
ATOM	3820	H2	H2O	31	29.640	60.183	42.110	1.00	0.00	W
ATOM	3821	OH2	H2O	32	28.197	52.345	43.775	1.00	24.75	W
ATOM	3822	H1	H2O	32	28.094	52.722	42.902	1.00	0.00	W
ATOM	3823	H2	H2O	32	28.541	51.469	43.622	1.00	0.00	W
ATOM	3824	OH2	H2O	33	23.054	77.785	-19.613	1.00	54.17	W
ATOM	3825	H1	H2O	33	23.018	77.086	-20.264	1.00	0.00	W
ATOM	3826	H2	H2O	33	23.144	78.588	-20.124	1.00	0.00	W
ATOM	3827	OH2	H2O	34	11.508	89.358	-0.033	1.00	89.65	W
ATOM	3828	H1	H2O	34	10.947	90.015	0.378	1.00	0.00	W
ATOM	3829	H2	H2O	34	11.860	88.850	0.697	1.00	0.00	W
ATOM	3830	OH2	H2O	35	11.641	45.393	37.448	1.00	51.14	W
ATOM	3831	H1	H2O	35	11.020	45.208	36.743	1.00	0.00	W
ATOM	3832	H2	H2O	35	11.965	44.531	37.713	1.00	0.00	W
ATOM	3833	OH2	H2O	36	20.569	40.000	37.790	1.00	29.17	W
ATOM	3834	H1	H2O	36	20.797	40.503	37.007	1.00	0.00	W
ATOM	3835	H2	H2O	36	20.901	40.523	38.517	1.00	0.00	W
ATOM	3836	OH2	H2O	37	24.685	71.120	-9.820	1.00	43.88	W
ATOM	3837	H1	H2O	37	25.328	70.841	-9.165	1.00	0.00	W
ATOM	3838	H2	H2O	37	24.632	70.379	-10.426	1.00	0.00	W
ATOM	3839	OH2	H2O	38	17.308	85.319	37.723	1.00	34.44	W
ATOM	3840	H1	H2O	38	18.044	85.879	37.954	1.00	0.00	W
ATOM	3841	H2	H2O	38	17.596	84.434	37.953	1.00	0.00	W
ATOM	3842	OH2	H2O	39	12.687	42.769	41.100	1.00	28.15	W
ATOM	3843	H1	H2O	39	12.510	41.844	40.940	1.00	0.00	W
ATOM	3844	H2	H2O	39	11.922	43.225	40.743	1.00	0.00	W
ATOM	3845	OH2	H2O	40	17.331	86.756	34.308	1.00	14.85	W
ATOM	3846	H1	H2O	40	18.021	87.306	34.677	1.00	0.00	W
ATOM	3847	H2	H2O	40	17.772	85.936	34.083	1.00	0.00	W
ATOM	3848	OH2	H2O	41	11.389	77.413	34.219	1.00	13.24	W
ATOM	3849	H1	H2O	41	11.834	76.632	33.886	1.00	0.00	W
ATOM	3850	H2	H2O	41	11.955	77.724	34.927	1.00	0.00	W
ATOM	3851	OH2	H2O	42	22.064	47.418	49.189	1.00	21.90	W
ATOM	3852	H1	H2O	42	22.578	47.067	49.916	1.00	0.00	W
ATOM	3853	H2	H2O	42	21.955	48.346	49.399	1.00	0.00	W
ATOM	3854	OH2	H2O	43	42.304	89.935	-4.829	1.00	41.26	W
ATOM	3855	H1	H2O	43	42.968	90.334	-4.263	1.00	0.00	W
ATOM	3856	H2	H2O	43	41.497	90.399	-4.614	1.00	0.00	W
ATOM	3857	OH2	H2O	44	20.332	50.701	49.638	1.00	34.52	W
ATOM	3858	H1	H2O	44	20.304	50.701	48.682	1.00	0.00	W
ATOM	3859	H2	H2O	44	20.709	51.553	49.866	1.00	0.00	W
ATOM	3860	OH2	H2O	45	29.753	79.163	20.128	1.00	29.41	W
ATOM	3861	H1	H2O	45	29.861	79.995	20.588	1.00	0.00	W
ATOM	3862	H2	H2O	45	30.517	78.646	20.388	1.00	0.00	W
ATOM	3863	OH2	H2O	46	21.428	84.063	13.081	1.00	37.53	W
ATOM	3864	H1	H2O	46	21.980	83.848	12.332	1.00	0.00	W
ATOM	3865	H2	H2O	46	22.024	84.033	13.833	1.00	0.00	W
ATOM	3866	OH2	H2O	47	44.014	87.180	0.493	1.00	42.34	W
ATOM	3867	H1	H2O	47	44.816	87.537	0.112	1.00	0.00	W
ATOM	3868	H2	H2O	47	44.255	86.949	1.390	1.00	0.00	W
ATOM	3869	OH2	H2O	48	10.349	58.686	20.367	1.00	54.51	W
ATOM	3870	H1	H2O	48	11.088	58.206	20.745	1.00	0.00	W
ATOM	3871	H2	H2O	48	10.744	59.467	19.982	1.00	0.00	W
ATOM	3872	OH2	H2O	50	23.990	56.220	51.509	1.00	25.41	W
ATOM	3873	H1	H2O	50	23.268	55.601	51.628	1.00	0.00	W
ATOM	3874	H2	H2O	50	24.178	56.195	50.573	1.00	0.00	W
ATOM	3875	OH2	H2O	51	14.872	75.264	-7.889	1.00	34.60	W
ATOM	3876	H1	H2O	51	15.737	75.461	-8.249	1.00	0.00	W
ATOM	3877	H2	H2O	51	15.004	75.262	-6.940	1.00	0.00	W

ATOM	3878	OH2	H2O	52	29.495	53.936	48.249	1.00	35.09	W
ATOM	3879	H1	H2O	52	30.382	53.691	48.511	1.00	0.00	W
ATOM	3880	H2	H2O	52	28.980	53.881	49.050	1.00	0.00	W
ATOM	3881	OH2	H2O	53	23.913	39.862	34.279	1.00	24.69	W
ATOM	3882	H1	H2O	53	23.928	40.573	34.917	1.00	0.00	W
ATOM	3883	H2	H2O	53	22.981	39.718	34.101	1.00	0.00	W
ATOM	3884	OH2	H2O	54	27.855	38.735	36.184	1.00	41.97	W
ATOM	3885	H1	H2O	54	27.501	37.874	35.965	1.00	0.00	W
ATOM	3886	H2	H2O	54	27.094	39.319	36.159	1.00	0.00	W
ATOM	3887	OH2	H2O	55	14.443	71.878	19.001	1.00	43.17	W
ATOM	3888	H1	H2O	55	13.698	71.493	18.533	1.00	0.00	W
ATOM	3889	H2	H2O	55	14.053	72.271	19.782	1.00	0.00	W
ATOM	3890	OH2	H2O	56	9.281	50.087	37.191	1.00	22.03	W
ATOM	3891	H1	H2O	56	10.124	49.922	36.769	1.00	0.00	W
ATOM	3892	H2	H2O	56	9.351	49.660	38.045	1.00	0.00	W
ATOM	3893	OH2	H2O	57	22.892	77.131	20.524	1.00	38.72	W
ATOM	3894	H1	H2O	57	22.303	76.460	20.869	1.00	0.00	W
ATOM	3895	H2	H2O	57	22.962	76.933	19.591	1.00	0.00	W
ATOM	3896	OH2	H2O	58	38.306	78.270	13.963	1.00	28.31	W
ATOM	3897	H1	H2O	58	38.886	77.518	14.102	1.00	0.00	W
ATOM	3898	H2	H2O	58	37.541	77.899	13.520	1.00	0.00	W
ATOM	3899	OH2	H2O	59	10.937	66.046	49.581	1.00	34.62	W
ATOM	3900	H1	H2O	59	11.082	66.814	49.032	1.00	0.00	W
ATOM	3901	H2	H2O	59	11.613	65.426	49.320	1.00	0.00	W
ATOM	3902	OH2	H2O	60	40.917	80.629	-4.294	1.00	39.29	W
ATOM	3903	H1	H2O	60	40.941	81.265	-5.010	1.00	0.00	W
ATOM	3904	H2	H2O	60	41.832	80.403	-4.141	1.00	0.00	W
ATOM	3905	OH2	H2O	61	37.462	76.032	26.379	1.00	35.75	W
ATOM	3906	H1	H2O	61	37.318	75.396	27.075	1.00	0.00	W
ATOM	3907	H2	H2O	61	36.637	76.059	25.897	1.00	0.00	W
ATOM	3908	OH2	H2O	62	12.194	92.917	7.443	1.00	26.35	W
ATOM	3909	H1	H2O	62	12.299	93.860	7.569	1.00	0.00	W
ATOM	3910	H2	H2O	62	12.553	92.749	6.576	1.00	0.00	W
ATOM	3911	OH2	H2O	63	10.746	48.472	38.472	1.00	32.24	W
ATOM	3912	H1	H2O	63	11.037	49.361	38.660	1.00	0.00	W
ATOM	3913	H2	H2O	63	11.406	47.907	38.868	1.00	0.00	W
ATOM	3914	OH2	H2O	64	24.609	73.773	41.569	1.00	29.16	W
ATOM	3915	H1	H2O	64	24.846	74.155	42.417	1.00	0.00	W
ATOM	3916	H2	H2O	64	25.433	73.754	41.081	1.00	0.00	W
ATOM	3917	OH2	H2O	65	30.012	66.185	-8.084	1.00	59.17	W
ATOM	3918	H1	H2O	65	30.800	66.596	-7.731	1.00	0.00	W
ATOM	3919	H2	H2O	65	29.658	66.832	-8.697	1.00	0.00	W
ATOM	3920	OH2	H2O	66	31.620	57.288	44.605	1.00	33.39	W
ATOM	3921	H1	H2O	66	30.791	56.867	44.837	1.00	0.00	W
ATOM	3922	H2	H2O	66	31.532	57.494	43.676	1.00	0.00	W
ATOM	3923	OH2	H2O	67	18.628	82.133	47.615	1.00	41.34	W
ATOM	3924	H1	H2O	67	19.144	81.345	47.779	1.00	0.00	W
ATOM	3925	H2	H2O	67	18.596	82.582	48.458	1.00	0.00	W
ATOM	3926	OH2	H2O	68	26.118	86.559	16.428	1.00	16.27	W
ATOM	3927	H1	H2O	68	25.731	86.540	17.305	1.00	0.00	W
ATOM	3928	H2	H2O	68	26.764	87.261	16.467	1.00	0.00	W
ATOM	3929	OH2	H2O	69	6.149	45.998	26.772	1.00	58.89	W
ATOM	3930	H1	H2O	69	6.523	46.223	27.625	1.00	0.00	W
ATOM	3931	H2	H2O	69	5.200	46.037	26.914	1.00	0.00	W
ATOM	3932	OH2	H2O	70	7.387	86.734	36.372	1.00	26.69	W
ATOM	3933	H1	H2O	70	7.690	87.232	35.613	1.00	0.00	W
ATOM	3934	H2	H2O	70	6.557	87.153	36.615	1.00	0.00	W
ATOM	3935	OH2	H2O	71	19.016	50.608	41.020	1.00	20.12	W
ATOM	3936	H1	H2O	71	19.744	51.094	41.405	1.00	0.00	W
ATOM	3937	H2	H2O	71	18.765	51.119	40.254	1.00	0.00	W
ATOM	3938	OH2	H2O	72	22.966	54.069	53.338	1.00	58.44	W
ATOM	3939	H1	H2O	72	22.736	53.762	54.218	1.00	0.00	W
ATOM	3940	H2	H2O	72	23.801	54.525	53.458	1.00	0.00	W
ATOM	3941	OH2	H2O	73	32.935	84.107	34.520	1.00	38.39	W
ATOM	3942	H1	H2O	73	32.932	85.062	34.520	1.00	0.00	W
ATOM	3943	H2	H2O	73	32.932	83.865	33.593	1.00	0.00	W
ATOM	3944	OH2	H2O	74	15.144	50.152	34.763	1.00	15.36	W
ATOM	3945	H1	H2O	74	15.994	49.728	34.642	1.00	0.00	W
ATOM	3946	H2	H2O	74	14.963	50.062	35.700	1.00	0.00	W
ATOM	3947	OH2	H2O	75	39.834	73.517	37.279	1.00	21.08	W
ATOM	3948	H1	H2O	75	39.093	73.212	37.805	1.00	0.00	W
ATOM	3949	H2	H2O	75	39.719	74.465	37.239	1.00	0.00	W
ATOM	3950	OH2	H2O	76	5.621	49.847	47.235	1.00	36.63	W

ATOM	3951	H1	H2O	76	5.682	50.181	48.127	1.00	0.00	W
ATOM	3952	H2	H2O	76	6.291	50.328	46.749	1.00	0.00	W
ATOM	3953	OH2	H2O	77	20.855	42.150	47.963	1.00	45.89	W
ATOM	3954	H1	H2O	77	21.782	42.249	47.739	1.00	0.00	W
ATOM	3955	H2	H2O	77	20.797	41.284	48.366	1.00	0.00	W
ATOM	3956	OH2	H2O	78	8.330	65.636	18.869	1.00	38.49	W
ATOM	3957	H1	H2O	78	8.581	66.186	18.125	1.00	0.00	W
ATOM	3958	H2	H2O	78	8.184	66.254	19.584	1.00	0.00	W
ATOM	3959	OH2	H2O	79	37.225	73.080	47.421	1.00	42.94	W
ATOM	3960	H1	H2O	79	37.775	72.667	46.755	1.00	0.00	W
ATOM	3961	H2	H2O	79	36.353	73.108	47.030	1.00	0.00	W
ATOM	3962	OH2	H2O	80	36.019	65.979	41.953	1.00	34.15	W
ATOM	3963	H1	H2O	80	36.913	65.996	42.303	1.00	0.00	W
ATOM	3964	H2	H2O	80	35.821	65.048	41.856	1.00	0.00	W
ATOM	3965	OH2	H2O	81	37.936	72.735	-2.902	1.00	58.65	W
ATOM	3966	H1	H2O	81	38.631	73.117	-2.367	1.00	0.00	W
ATOM	3967	H2	H2O	81	37.913	73.277	-3.690	1.00	0.00	W
ATOM	3968	OH2	H2O	82	23.143	50.854	55.229	1.00	73.08	W
ATOM	3969	H1	H2O	82	22.200	50.699	55.185	1.00	0.00	W
ATOM	3970	H2	H2O	82	23.429	50.377	56.008	1.00	0.00	W
ATOM	3971	OH2	H2O	83	35.270	96.894	-8.992	1.00	46.37	W
ATOM	3972	H1	H2O	83	34.385	97.082	-9.298	1.00	0.00	W
ATOM	3973	H2	H2O	83	35.800	97.621	-9.320	1.00	0.00	W
ATOM	3974	OH2	H2O	84	34.683	68.046	40.254	1.00	41.87	W
ATOM	3975	H1	H2O	84	35.001	67.185	39.981	1.00	0.00	W
ATOM	3976	H2	H2O	84	33.743	68.022	40.069	1.00	0.00	W
ATOM	3977	OH2	H2O	85	7.937	93.884	8.479	1.00	67.26	W
ATOM	3978	H1	H2O	85	8.505	93.128	8.331	1.00	0.00	W
ATOM	3979	H2	H2O	85	7.793	94.250	7.607	1.00	0.00	W
ATOM	3980	OH2	H2O	86	41.437	88.270	5.694	1.00	43.07	W
ATOM	3981	H1	H2O	86	40.650	88.680	6.057	1.00	0.00	W
ATOM	3982	H2	H2O	86	41.183	87.355	5.556	1.00	0.00	W
ATOM	3983	OH2	H2O	87	18.418	89.968	41.295	1.00	50.98	W
ATOM	3984	H1	H2O	87	19.346	89.974	41.525	1.00	0.00	W
ATOM	3985	H2	H2O	87	18.287	89.127	40.854	1.00	0.00	W
ATOM	3986	OH2	H2O	88	15.346	97.033	5.772	1.00	51.64	W
ATOM	3987	H1	H2O	88	14.535	97.052	5.262	1.00	0.00	W
ATOM	3988	H2	H2O	88	15.780	96.224	5.502	1.00	0.00	W
ATOM	3989	OH2	H2O	89	47.753	89.370	-3.781	1.00	37.41	W
ATOM	3990	H1	H2O	89	47.756	90.330	-3.781	1.00	0.00	W
ATOM	3991	H2	H2O	89	47.756	89.133	-4.708	1.00	0.00	W
ATOM	3992	OH2	H2O	90	17.822	70.217	21.038	1.00	53.57	W
ATOM	3993	H1	H2O	90	18.493	70.890	21.166	1.00	0.00	W
ATOM	3994	H2	H2O	90	17.151	70.426	21.692	1.00	0.00	W
ATOM	3995	OH2	H2O	91	2.696	51.590	41.944	1.00	46.78	W
ATOM	3996	H1	H2O	91	1.893	51.743	42.439	1.00	0.00	W
ATOM	3997	H2	H2O	91	3.400	51.837	42.544	1.00	0.00	W
ATOM	3998	OH2	H2O	95	34.676	75.860	41.073	1.00	39.50	W
ATOM	3999	H1	H2O	95	35.228	75.793	40.290	1.00	0.00	W
ATOM	4000	H2	H2O	95	34.453	74.957	41.286	1.00	0.00	W
ATOM	4001	OH2	H2O	96	39.675	76.625	-9.371	1.00	56.41	W
ATOM	4002	H1	H2O	96	38.896	76.095	-9.211	1.00	0.00	W
ATOM	4003	H2	H2O	96	40.385	75.984	-9.456	1.00	0.00	W
ATOM	4004	OH2	H2O	97	18.254	64.042	7.803	1.00	55.42	W
ATOM	4005	H1	H2O	97	18.067	64.981	7.768	1.00	0.00	W
ATOM	4006	H2	H2O	97	17.406	63.636	7.982	1.00	0.00	W
ATOM	4007	OH2	H2O	99	36.040	76.842	46.828	1.00	41.76	W
ATOM	4008	H1	H2O	99	35.612	76.180	46.290	1.00	0.00	W
ATOM	4009	H2	H2O	99	35.367	77.514	46.962	1.00	0.00	W
ATOM	4010	OH2	H2O	100	39.087	90.744	-12.653	1.00	50.93	W
ATOM	4011	H1	H2O	100	39.148	91.213	-13.482	1.00	0.00	W
ATOM	4012	H2	H2O	100	39.394	91.370	-11.997	1.00	0.00	W
ATOM	4013	OH2	H2O	102	34.315	73.486	18.013	1.00	32.56	W
ATOM	4014	H1	H2O	102	34.941	73.597	17.299	1.00	0.00	W
ATOM	4015	H2	H2O	102	33.483	73.303	17.577	1.00	0.00	W
ATOM	4016	OH2	H2O	103	27.629	65.918	7.501	1.00	26.86	W
ATOM	4017	H1	H2O	103	26.981	65.607	8.130	1.00	0.00	W
ATOM	4018	H2	H2O	103	28.387	65.342	7.634	1.00	0.00	W
ATOM	4019	OH2	H2O	104	30.549	69.755	-10.939	1.00	52.39	W
ATOM	4020	H1	H2O	104	30.082	70.440	-11.415	1.00	0.00	W
ATOM	4021	H2	H2O	104	30.530	68.998	-11.524	1.00	0.00	W
ATOM	4022	OH2	H2O	105	34.538	71.979	38.560	1.00	30.69	W
ATOM	4023	H1	H2O	105	33.720	72.302	38.185	1.00	0.00	W

ATOM	4024	H2	H2O	105	34.317	71.734	39.455	1.00	0.00	W
ATOM	4025	OH2	H2O	106	31.168	67.923	13.585	1.00	47.02	W
ATOM	4026	H1	H2O	106	31.193	67.876	14.540	1.00	0.00	W
ATOM	4027	H2	H2O	106	30.514	68.599	13.396	1.00	0.00	W
ATOM	4028	OH2	H2O	107	32.794	63.732	44.548	1.00	33.54	W
ATOM	4029	H1	H2O	107	32.546	63.550	45.458	1.00	0.00	W
ATOM	4030	H2	H2O	107	33.687	63.411	44.472	1.00	0.00	W
ATOM	4031	OH2	H2O	108	19.475	88.576	35.346	1.00	35.25	W
ATOM	4032	H1	H2O	108	19.617	88.129	34.508	1.00	0.00	W
ATOM	4033	H2	H2O	108	20.226	88.319	35.881	1.00	0.00	W
ATOM	4034	OH2	H2O	109	23.864	52.354	23.080	1.00	48.58	W
ATOM	4035	H1	H2O	109	23.166	52.051	22.499	1.00	0.00	W
ATOM	4036	H2	H2O	109	23.422	52.922	23.711	1.00	0.00	W
ATOM	4037	OH2	H2O	110	31.956	52.640	32.308	1.00	51.66	W
ATOM	4038	H1	H2O	110	31.785	52.563	31.371	1.00	0.00	W
ATOM	4039	H2	H2O	110	31.086	52.644	32.711	1.00	0.00	W
ATOM	4040	OH2	H2O	111	16.968	60.681	13.605	1.00	55.65	W
ATOM	4041	H1	H2O	111	16.618	60.785	12.718	1.00	0.00	W
ATOM	4042	H2	H2O	111	17.849	61.054	13.557	1.00	0.00	W
ATOM	4043	OH2	H2O	112	38.699	63.142	37.584	1.00	49.09	W
ATOM	4044	H1	H2O	112	37.844	62.845	37.265	1.00	0.00	W
ATOM	4045	H2	H2O	112	39.233	62.347	37.604	1.00	0.00	W
ATOM	4046	OH2	H2O	113	31.344	57.427	39.398	1.00	37.73	W
ATOM	4047	H1	H2O	113	31.126	56.895	40.166	1.00	0.00	W
ATOM	4048	H2	H2O	113	30.552	57.933	39.226	1.00	0.00	W
ATOM	4049	OH2	H2O	114	41.350	83.449	-8.714	1.00	60.04	W
ATOM	4050	H1	H2O	114	41.043	83.752	-9.569	1.00	0.00	W
ATOM	4051	H2	H2O	114	41.072	84.130	-8.103	1.00	0.00	W
ATOM	4052	OH2	H2O	115	42.987	90.912	5.698	1.00	36.99	W
ATOM	4053	H1	H2O	115	42.742	89.993	5.572	1.00	0.00	W
ATOM	4054	H2	H2O	115	43.930	90.888	5.853	1.00	0.00	W
ATOM	4055	OH2	H2O	118	27.240	71.465	53.783	1.00	33.44	W
ATOM	4056	H1	H2O	118	27.239	72.422	53.780	1.00	0.00	W
ATOM	4057	H2	H2O	118	27.239	71.225	52.853	1.00	0.00	W
ATOM	4058	OH2	H2O	119	11.225	50.304	22.316	1.00	55.33	W
ATOM	4059	H1	H2O	119	11.185	51.196	22.657	1.00	0.00	W
ATOM	4060	H2	H2O	119	10.758	50.343	21.483	1.00	0.00	W
ATOM	4061	OH2	H2O	122	10.516	74.345	13.709	1.00	49.01	W
ATOM	4062	H1	H2O	122	11.305	74.880	13.770	1.00	0.00	W
ATOM	4063	H2	H2O	122	10.747	73.529	14.153	1.00	0.00	W
ATOM	4064	OH2	H2O	123	21.221	81.929	43.450	1.00	35.78	W
ATOM	4065	H1	H2O	123	20.410	82.390	43.227	1.00	0.00	W
ATOM	4066	H2	H2O	123	21.623	82.469	44.129	1.00	0.00	W
ATOM	4067	OH2	H2O	125	26.901	87.147	37.889	1.00	67.29	W
ATOM	4068	H1	H2O	125	25.985	87.057	37.631	1.00	0.00	W
ATOM	4069	H2	H2O	125	26.955	86.709	38.739	1.00	0.00	W
ATOM	4070	OH2	H2O	127	38.005	73.517	7.577	1.00	47.94	W
ATOM	4071	H1	H2O	127	38.835	73.559	7.101	1.00	0.00	W
ATOM	4072	H2	H2O	127	38.249	73.253	8.463	1.00	0.00	W
ATOM	4073	OH2	H2O	130	10.402	70.971	29.298	1.00	20.65	W
ATOM	4074	H1	H2O	130	9.723	71.264	28.687	1.00	0.00	W
ATOM	4075	H2	H2O	130	10.159	71.385	30.132	1.00	0.00	W
ATOM	4076	OH2	H2O	132	5.650	81.404	36.223	1.00	27.14	W
ATOM	4077	H1	H2O	132	4.752	81.595	36.500	1.00	0.00	W
ATOM	4078	H2	H2O	132	6.195	81.776	36.918	1.00	0.00	W
ATOM	4079	OH2	H2O	133	13.263	68.119	49.513	1.00	44.60	W
ATOM	4080	H1	H2O	133	13.357	67.240	49.144	1.00	0.00	W
ATOM	4081	H2	H2O	133	13.500	68.707	48.799	1.00	0.00	W
ATOM	4082	OH2	H2O	134	19.524	87.618	-11.380	1.00	25.22	W
ATOM	4083	H1	H2O	134	19.588	86.908	-10.742	1.00	0.00	W
ATOM	4084	H2	H2O	134	18.725	87.424	-11.875	1.00	0.00	W
ATOM	4085	OH2	H2O	135	40.212	59.845	25.750	1.00	51.43	W
ATOM	4086	H1	H2O	135	41.124	59.975	26.015	1.00	0.00	W
ATOM	4087	H2	H2O	135	40.235	59.869	24.793	1.00	0.00	W
ATOM	4088	OH2	H2O	136	19.922	100.636	-9.493	1.00	47.67	W
ATOM	4089	H1	H2O	136	19.113	101.141	-9.422	1.00	0.00	W
ATOM	4090	H2	H2O	136	20.620	101.276	-9.363	1.00	0.00	W
ATOM	4091	OH2	H2O	137	7.532	75.485	18.573	1.00	47.00	W
ATOM	4092	H1	H2O	137	7.714	76.396	18.784	1.00	0.00	W
ATOM	4093	H2	H2O	137	6.759	75.513	18.008	1.00	0.00	W
ATOM	4094	OH2	H2O	139	25.465	59.184	52.290	1.00	28.76	W
ATOM	4095	H1	H2O	139	25.749	59.465	51.420	1.00	0.00	W
ATOM	4096	H2	H2O	139	24.512	59.318	52.281	1.00	0.00	W

ATOM	4097	OH2	H2O	140	14.960	69.189	7.890	1.00	46.58	W
ATOM	4098	H1	H2O	140	14.139	69.668	7.972	1.00	0.00	W
ATOM	4099	H2	H2O	140	15.631	69.867	7.811	1.00	0.00	W
ATOM	4100	OH2	H2O	142	31.562	73.845	26.725	1.00	46.85	W
ATOM	4101	H1	H2O	142	30.757	74.357	26.741	1.00	0.00	W
ATOM	4102	H2	H2O	142	31.916	73.978	25.843	1.00	0.00	W
ATOM	4103	OH2	H2O	143	24.525	81.714	35.572	1.00	45.84	W
ATOM	4104	H1	H2O	143	23.681	81.414	35.237	1.00	0.00	W
ATOM	4105	H2	H2O	143	25.142	81.535	34.862	1.00	0.00	W
ATOM	4106	OH2	H2O	144	30.404	37.547	38.155	1.00	49.49	W
ATOM	4107	H1	H2O	144	31.040	37.919	38.772	1.00	0.00	W
ATOM	4108	H2	H2O	144	29.868	38.295	37.890	1.00	0.00	W
ATOM	4109	OH2	H2O	145	18.510	37.954	48.005	1.00	31.26	W
ATOM	4110	H1	H2O	145	18.573	37.366	48.753	1.00	0.00	W
ATOM	4111	H2	H2O	145	19.251	37.719	47.448	1.00	0.00	W
ATOM	4112	OH2	H2O	148	21.454	103.453	-11.072	1.00	69.13	W
ATOM	4113	H1	H2O	148	21.532	103.913	-10.238	1.00	0.00	W
ATOM	4114	H2	H2O	148	20.530	103.207	-11.127	1.00	0.00	W
ATOM	4115	OH2	H2O	149	30.616	69.892	11.062	1.00	59.13	W
ATOM	4116	H1	H2O	149	30.597	69.088	10.544	1.00	0.00	W
ATOM	4117	H2	H2O	149	31.534	69.990	11.317	1.00	0.00	W
ATOM	4118	OH2	H2O	151	22.397	96.000	-18.890	1.00	49.14	W
ATOM	4119	H1	H2O	151	22.660	96.162	-19.796	1.00	0.00	W
ATOM	4120	H2	H2O	151	22.588	95.071	-18.750	1.00	0.00	W
ATOM	4121	OH2	H2O	152	23.997	68.719	-3.081	1.00	37.05	W
ATOM	4122	H1	H2O	152	23.944	69.622	-3.393	1.00	0.00	W
ATOM	4123	H2	H2O	152	23.498	68.717	-2.264	1.00	0.00	W
ATOM	4124	OH2	H2O	153	6.761	78.049	41.002	1.00	44.92	W
ATOM	4125	H1	H2O	153	6.495	77.572	40.213	1.00	0.00	W
ATOM	4126	H2	H2O	153	7.695	77.879	41.080	1.00	0.00	W
ATOM	4127	OH2	H2O	154	14.604	84.085	47.918	1.00	27.17	W
ATOM	4128	H1	H2O	154	14.800	83.921	48.839	1.00	0.00	W
ATOM	4129	H2	H2O	154	15.458	84.196	47.504	1.00	0.00	W
ATOM	4130	OH2	H2O	157	20.208	87.608	38.773	1.00	46.36	W
ATOM	4131	H1	H2O	157	19.447	88.077	38.424	1.00	0.00	W
ATOM	4132	H2	H2O	157	20.838	88.299	38.980	1.00	0.00	W
ATOM	4133	OH2	H2O	161	27.786	81.756	30.433	1.00	20.04	W
ATOM	4134	H1	H2O	161	27.657	81.992	31.345	1.00	0.00	W
ATOM	4135	H2	H2O	161	27.013	81.230	30.207	1.00	0.00	W
ATOM	4136	OH2	H2O	162	25.545	41.107	41.204	1.00	39.67	W
ATOM	4137	H1	H2O	162	26.123	40.371	41.410	1.00	0.00	W
ATOM	4138	H2	H2O	162	24.668	40.789	41.410	1.00	0.00	W
ATOM	4139	OH2	H2O	163	34.968	61.130	39.718	1.00	58.53	W
ATOM	4140	H1	H2O	163	35.625	61.220	40.410	1.00	0.00	W
ATOM	4141	H2	H2O	163	34.194	60.792	40.166	1.00	0.00	W
ATOM	4142	OH2	H2O	164	31.867	61.174	40.931	1.00	30.31	W
ATOM	4143	H1	H2O	164	31.027	60.812	40.654	1.00	0.00	W
ATOM	4144	H2	H2O	164	31.803	61.239	41.882	1.00	0.00	W
ATOM	4145	OH2	H2O	165	18.529	51.777	47.785	1.00	26.36	W
ATOM	4146	H1	H2O	165	18.240	52.561	48.263	1.00	0.00	W
ATOM	4147	H2	H2O	165	18.619	51.109	48.456	1.00	0.00	W
ATOM	4148	OH2	H2O	166	6.824	56.798	46.694	1.00	31.23	W
ATOM	4149	H1	H2O	166	7.339	56.878	47.493	1.00	0.00	W
ATOM	4150	H2	H2O	166	5.921	56.982	46.973	1.00	0.00	W
ATOM	4151	OH2	H2O	167	4.124	74.966	21.486	1.00	35.69	W
ATOM	4152	H1	H2O	167	4.300	75.262	20.590	1.00	0.00	W
ATOM	4153	H2	H2O	167	4.736	75.467	22.026	1.00	0.00	W
ATOM	4154	OH2	H2O	168	23.115	81.286	-19.644	1.00	56.66	W
ATOM	4155	H1	H2O	168	23.431	81.070	-20.521	1.00	0.00	W
ATOM	4156	H2	H2O	168	23.194	80.469	-19.152	1.00	0.00	W
ATOM	4157	OH2	H2O	169	3.381	70.239	27.505	1.00	32.76	W
ATOM	4158	H1	H2O	169	2.709	70.126	26.830	1.00	0.00	W
ATOM	4159	H2	H2O	169	3.950	70.929	27.161	1.00	0.00	W
ATOM	4160	OH2	H2O	170	38.354	96.654	-4.019	1.00	38.96	W
ATOM	4161	H1	H2O	170	38.897	97.181	-4.602	1.00	0.00	W
ATOM	4162	H2	H2O	170	38.910	95.925	-3.757	1.00	0.00	W
ATOM	4163	OH2	H2O	171	31.765	75.253	24.200	1.00	35.79	W
ATOM	4164	H1	H2O	171	31.801	76.033	23.651	1.00	0.00	W
ATOM	4165	H2	H2O	171	32.622	74.840	24.093	1.00	0.00	W
ATOM	4166	OH2	H2O	172	30.112	51.159	46.701	1.00	42.99	W
ATOM	4167	H1	H2O	172	29.550	51.828	47.094	1.00	0.00	W
ATOM	4168	H2	H2O	172	30.504	50.708	47.449	1.00	0.00	W
ATOM	4169	OH2	H2O	173	14.724	60.204	54.146	1.00	44.12	W

ATOM	4170	H1	H2O	173	13.852	60.500	54.408	1.00	0.00	W
ATOM	4171	H2	H2O	173	15.149	59.955	54.966	1.00	0.00	W
ATOM	4172	OH2	H2O	174	34.426	92.105	20.174	1.00	43.09	W
ATOM	4173	H1	H2O	174	33.995	92.193	19.323	1.00	0.00	W
ATOM	4174	H2	H2O	174	35.110	92.775	20.165	1.00	0.00	W
ATOM	4175	OH2	H2O	175	15.079	77.472	19.106	1.00	26.05	W
ATOM	4176	H1	H2O	175	15.197	78.034	19.868	1.00	0.00	W
ATOM	4177	H2	H2O	175	14.807	76.627	19.465	1.00	0.00	W
ATOM	4178	OH2	H2O	176	4.428	65.813	39.483	1.00	41.04	W
ATOM	4179	H1	H2O	176	4.482	66.597	38.935	1.00	0.00	W
ATOM	4180	H2	H2O	176	3.948	66.099	40.261	1.00	0.00	W
ATOM	4181	OH2	H2O	177	15.709	70.351	-5.398	1.00	60.42	W
ATOM	4182	H1	H2O	177	15.048	70.541	-4.731	1.00	0.00	W
ATOM	4183	H2	H2O	177	15.488	69.475	-5.712	1.00	0.00	W
ATOM	4184	OH2	H2O	178	33.370	76.092	46.298	1.00	73.91	W
ATOM	4185	H1	H2O	178	32.527	75.849	46.680	1.00	0.00	W
ATOM	4186	H2	H2O	178	33.647	76.862	46.791	1.00	0.00	W
ATOM	4187	OH2	H2O	179	32.160	88.256	-3.330	1.00	31.03	W
ATOM	4188	H1	H2O	179	31.330	88.041	-3.759	1.00	0.00	W
ATOM	4189	H2	H2O	179	32.571	88.893	-3.916	1.00	0.00	W
ATOM	4190	OH2	H2O	180	43.785	91.145	1.609	1.00	42.82	W
ATOM	4191	H1	H2O	180	44.441	91.779	1.325	1.00	0.00	W
ATOM	4192	H2	H2O	180	44.208	90.654	2.311	1.00	0.00	W
ATOM	4193	OH2	H2O	181	23.220	65.998	2.718	1.00	25.59	W
ATOM	4194	H1	H2O	181	22.845	66.784	2.330	1.00	0.00	W
ATOM	4195	H2	H2O	181	22.846	65.275	2.212	1.00	0.00	W
ATOM	4196	OH2	H2O	182	7.003	43.420	24.621	1.00	50.96	W
ATOM	4197	H1	H2O	182	7.061	43.954	25.414	1.00	0.00	W
ATOM	4198	H2	H2O	182	7.912	43.254	24.376	1.00	0.00	W
ATOM	4199	OH2	H2O	183	27.129	44.901	42.342	1.00	61.07	W
ATOM	4200	H1	H2O	183	26.349	45.392	42.607	1.00	0.00	W
ATOM	4201	H2	H2O	183	27.383	44.415	43.126	1.00	0.00	W
ATOM	4202	OH2	H2O	184	20.120	62.615	6.341	1.00	52.42	W
ATOM	4203	H1	H2O	184	19.717	63.462	6.535	1.00	0.00	W
ATOM	4204	H2	H2O	184	20.224	62.197	7.197	1.00	0.00	W
ATOM	4205	OH2	H2O	186	10.038	94.189	-8.999	1.00	40.69	W
ATOM	4206	H1	H2O	186	10.000	93.361	-9.481	1.00	0.00	W
ATOM	4207	H2	H2O	186	9.190	94.600	-9.161	1.00	0.00	W
ATOM	4208	OH2	H2O	187	39.048	78.109	48.627	1.00	43.94	W
ATOM	4209	H1	H2O	187	39.049	79.067	48.627	1.00	0.00	W
ATOM	4210	H2	H2O	187	39.049	77.870	47.700	1.00	0.00	W
ATOM	4211	OH2	H2O	188	29.997	88.546	37.175	1.00	66.02	W
ATOM	4212	H1	H2O	188	29.998	89.503	37.176	1.00	0.00	W
ATOM	4213	H2	H2O	188	29.998	88.306	36.249	1.00	0.00	W
ATOM	4214	OH2	H2O	189	33.213	66.563	16.332	1.00	62.88	W
ATOM	4215	H1	H2O	189	33.911	66.201	15.788	1.00	0.00	W
ATOM	4216	H2	H2O	189	33.092	67.455	16.008	1.00	0.00	W
ATOM	4217	OH2	H2O	190	29.894	60.575	22.671	1.00	41.27	W
ATOM	4218	H1	H2O	190	29.363	61.361	22.549	1.00	0.00	W
ATOM	4219	H2	H2O	190	30.767	60.909	22.889	1.00	0.00	W
ATOM	4220	OH2	H2O	191	17.276	53.069	43.250	1.00	10.66	W
ATOM	4221	H1	H2O	191	17.592	53.312	44.119	1.00	0.00	W
ATOM	4222	H2	H2O	191	18.045	52.689	42.817	1.00	0.00	W
ATOM	4223	OH2	H2O	192	35.647	59.655	27.750	1.00	26.14	W
ATOM	4224	H1	H2O	192	36.404	59.816	28.311	1.00	0.00	W
ATOM	4225	H2	H2O	192	35.899	60.010	26.897	1.00	0.00	W
ATOM	4226	OH2	H2O	193	38.775	60.787	30.053	1.00	36.89	W
ATOM	4227	H1	H2O	193	38.108	61.130	29.455	1.00	0.00	W
ATOM	4228	H2	H2O	193	39.557	61.302	29.857	1.00	0.00	W
ATOM	4229	OH2	H2O	194	18.790	80.718	52.778	1.00	28.10	W
ATOM	4230	H1	H2O	194	18.791	81.672	52.780	1.00	0.00	W
ATOM	4231	H2	H2O	194	18.791	80.475	51.853	1.00	0.00	W
ATOM	4232	OH2	H2O	195	22.571	68.265	53.229	1.00	34.42	W
ATOM	4233	H1	H2O	195	23.152	67.936	53.916	1.00	0.00	W
ATOM	4234	H2	H2O	195	22.266	69.110	53.558	1.00	0.00	W
ATOM	4235	OH2	H2O	196	7.904	98.993	-8.160	1.00	39.75	W
ATOM	4236	H1	H2O	196	7.904	99.952	-8.160	1.00	0.00	W
ATOM	4237	H2	H2O	196	7.904	98.755	-9.087	1.00	0.00	W
ATOM	4238	OH2	H2O	197	15.117	76.593	49.958	1.00	44.24	W
ATOM	4239	H1	H2O	197	14.700	76.989	50.724	1.00	0.00	W
ATOM	4240	H2	H2O	197	15.264	77.325	49.360	1.00	0.00	W
ATOM	4241	OH2	H2O	198	18.738	61.062	5.012	1.00	57.29	W
ATOM	4242	H1	H2O	198	18.739	62.019	5.011	1.00	0.00	W

	ATOM	4243	H2	H2O	198	18.739	60.822	4.084	1.00	0.00	W
	ATOM	4244	OH2	H2O	199	38.023	88.017	8.921	1.00	34.68	W
	ATOM	4245	H1	H2O	199	37.201	88.224	9.366	1.00	0.00	W
	ATOM	4246	H2	H2O	199	37.785	87.348	8.278	1.00	0.00	W
5	ATOM	4247	OH2	H2O	200	25.176	78.050	39.750	1.00	36.28	W
	ATOM	4248	H1	H2O	200	25.349	78.069	38.807	1.00	0.00	W
	ATOM	4249	H2	H2O	200	24.306	78.440	39.840	1.00	0.00	W
	ATOM	4250	OH2	H2O	201	36.509	75.837	18.830	1.00	40.11	W
	ATOM	4251	H1	H2O	201	36.944	75.281	19.473	1.00	0.00	W
10	ATOM	4252	H2	H2O	201	36.226	76.605	19.326	1.00	0.00	W
	ATOM	4253	OH2	H2O	202	15.114	86.425	44.318	1.00	26.14	W
	ATOM	4254	H1	H2O	202	14.743	86.504	43.441	1.00	0.00	W
	ATOM	4255	H2	H2O	202	15.979	86.832	44.251	1.00	0.00	W
	ATOM	4256	OH2	H2O	203	34.096	66.512	23.788	1.00	48.56	W
15	ATOM	4257	H1	H2O	203	34.012	66.195	24.690	1.00	0.00	W
	ATOM	4258	H2	H2O	203	34.943	66.959	23.773	1.00	0.00	W
	ATOM	4259	OH2	H2O	204	28.998	83.540	37.915	1.00	48.28	W
	ATOM	4260	H1	H2O	204	29.160	83.028	37.122	1.00	0.00	W
	ATOM	4261	H2	H2O	204	29.874	83.729	38.257	1.00	0.00	W
20	ATOM	4262	OH2	H2O	205	36.771	86.241	17.583	1.00	28.64	W
	ATOM	4263	H1	H2O	205	37.720	86.287	17.698	1.00	0.00	W
	ATOM	4264	H2	H2O	205	36.608	86.681	16.750	1.00	0.00	W
	ATOM	4265	OH2	H2O	206	34.304	83.977	22.394	1.00	37.11	W
	ATOM	4266	H1	H2O	206	33.908	83.964	23.266	1.00	0.00	W
25	ATOM	4267	H2	H2O	206	33.588	84.238	21.812	1.00	0.00	W
	ATOM	4268	OH2	H2O	207	10.426	85.642	38.336	1.00	35.00	W
	ATOM	4269	H1	H2O	207	10.276	85.151	39.144	1.00	0.00	W
	ATOM	4270	H2	H2O	207	10.589	86.537	38.626	1.00	0.00	W
	ATOM	4271	OH2	H2O	208	33.164	40.493	36.564	1.00	43.55	W
30	ATOM	4272	H1	H2O	208	33.931	39.992	36.285	1.00	0.00	W
	ATOM	4273	H2	H2O	208	32.453	40.170	36.012	1.00	0.00	W
	ATOM	4274	OH2	H2O	209	9.667	59.806	49.799	1.00	27.66	W
	ATOM	4275	H1	H2O	209	9.078	59.514	49.107	1.00	0.00	W
	ATOM	4276	H2	H2O	209	10.523	59.452	49.554	1.00	0.00	W
35	ATOM	4277	OH2	H2O	210	40.620	91.683	9.844	1.00	44.74	W
	ATOM	4278	H1	H2O	210	39.757	91.357	10.104	1.00	0.00	W
	ATOM	4279	H2	H2O	210	40.905	91.080	9.157	1.00	0.00	W
	ATOM	4280	OH2	H2O	211	31.114	53.143	38.106	1.00	19.43	W
	ATOM	4281	H1	H2O	211	30.669	52.292	38.079	1.00	0.00	W
40	ATOM	4282	H2	H2O	211	31.806	53.073	37.457	1.00	0.00	W
	ATOM	4283	OH2	H2O	212	37.410	58.585	24.168	1.00	51.69	W
	ATOM	4284	H1	H2O	212	36.615	59.088	23.990	1.00	0.00	W
	ATOM	4285	H2	H2O	212	37.097	57.750	24.508	1.00	0.00	W
	ATOM	4286	OH2	H2O	213	37.530	82.337	17.584	1.00	25.73	W
45	ATOM	4287	H1	H2O	213	36.642	81.987	17.649	1.00	0.00	W
	ATOM	4288	H2	H2O	213	38.090	81.564	17.520	1.00	0.00	W
	ATOM	4289	OH2	H2O	214	20.562	62.057	49.243	1.00	36.13	W
	ATOM	4290	H1	H2O	214	20.191	62.888	48.941	1.00	0.00	W
	ATOM	4291	H2	H2O	214	20.159	61.398	48.677	1.00	0.00	W
50	ATOM	4292	OH2	H2O	215	38.487	67.744	46.984	1.00	28.08	W
	ATOM	4293	H1	H2O	215	38.487	68.698	46.981	1.00	0.00	W
	ATOM	4294	H2	H2O	215	38.487	67.501	46.054	1.00	0.00	W
	ATOM	4295	OH2	H2O	216	4.672	50.241	43.410	1.00	37.85	W
	ATOM	4296	H1	H2O	216	3.799	49.905	43.616	1.00	0.00	W
55	ATOM	4297	H2	H2O	216	5.068	50.420	44.262	1.00	0.00	W
	ATOM	4298	OH2	H2O	217	32.087	71.911	7.975	1.00	35.72	W
	ATOM	4299	H1	H2O	217	32.492	72.674	7.563	1.00	0.00	W
	ATOM	4300	H2	H2O	217	31.862	72.205	8.857	1.00	0.00	W
	ATOM	4301	OH2	H2O	218	37.077	71.241	31.371	1.00	28.59	W
60	ATOM	4302	H1	H2O	218	36.181	71.414	31.087	1.00	0.00	W
	ATOM	4303	H2	H2O	218	37.354	70.488	30.847	1.00	0.00	W
	ATOM	4304	OH2	H2O	219	12.531	78.336	47.863	1.00	38.31	W
	ATOM	4305	H1	H2O	219	11.632	78.370	47.538	1.00	0.00	W
	ATOM	4306	H2	H2O	219	12.440	78.304	48.816	1.00	0.00	W
65	ATOM	4307	OH2	H2O	236	5.922	55.713	49.951	1.00	34.41	W
	ATOM	4308	H1	H2O	236	6.664	55.901	49.382	1.00	0.00	W
	ATOM	4309	H2	H2O	236	6.297	55.224	50.679	1.00	0.00	W
	ATOM	4310	OH2	H2O	237	32.810	50.612	40.203	1.00	42.20	W
	ATOM	4311	H1	H2O	237	32.021	51.115	40.399	1.00	0.00	W
70	ATOM	4312	H2	H2O	237	32.497	49.728	40.026	1.00	0.00	W
	ATOM	4313	OH2	H2O	238	16.579	101.122	-4.447	1.00	38.51	W
	ATOM	4314	H1	H2O	238	15.993	101.299	-5.184	1.00	0.00	W
	ATOM	4315	H2	H2O	238	16.974	100.276	-4.652	1.00	0.00	W

ATOM	4316	OH2	H2O	239	17.874	69.091	56.692	1.00	38.94	W
ATOM	4317	H1	H2O	239	17.874	70.049	56.691	1.00	0.00	W
ATOM	4318	H2	H2O	239	17.874	68.852	55.764	1.00	0.00	W
ATOM	4319	OH2	H2O	240	12.249	77.436	-11.341	1.00	40.18	W
ATOM	4320	H1	H2O	240	12.960	78.076	-11.282	1.00	0.00	W
ATOM	4321	H2	H2O	240	12.370	77.023	-12.196	1.00	0.00	W
ATOM	4322	OH2	H2O	241	29.087	65.635	23.981	1.00	33.57	W
ATOM	4323	H1	H2O	241	28.790	65.725	24.885	1.00	0.00	W
ATOM	4324	H2	H2O	241	29.863	66.198	23.928	1.00	0.00	W